Fast and accurate computation of Jacobi expansion coefficients of analytic functions

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The computation of spectral expansion coefficients is an important aspect in the implementation of spectral methods. In this paper, we explore two strategies for computing the coefficients of polynomial expansions of analytic functions, including Chebyshev, Legendre, ultraspherical and Jacobi coefficients, in the complex plane. The first strategy maximizes computational efficiency and results in an FFT-based $\mathcal{O}(\mathcal{N} \log \mathcal{N})$ algorithm for computing the first N spectral expansion coefficients. This strategy is stable with respect to absolute errors and recovers some recent algorithms for the computation of Legendre and ultraspherical spectral coefficients as special cases. The second strategy maximizes computational accuracy. We show that an optimal contour in the complex plane exists for each Chebyshev expansion coefficient. With these contours Chebyshev coefficients can be computed with small relative error, rather than the usual small absolute error, at a cost of increasing the computational complexity. We show that high accuracy is maintained even after repeated differentiation of the expansion, such that very high order derivatives of analytic functions can be computed to near machine precision accuracy from their Chebyshev expansions using standard floating point arithmetic. This result is similar to a result recently obtained by Bornemann for the computation of high order derivatives by Cauchy integrals. We extend this strategy to the accurate computation of Jacobi coefficients.

Keywords : spectral expansion, analytic functions, Jacobi polynomials, FFT
AMS(MOS) Classification : Primary : 42C10, Secondary : 65N35.

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1 Introduction

The Jacobi polynomials, along with their special cases the Legendre, Chebyshev and ultraspherical or Gegenbauer polynomials, are widely used in many fields of numerical analysis such as approximation theory, the construction of Gauss-type quadrature formulae, spectral methods for ordinary and partial differential equations [19], the resolution of the Gibbs phenomenon [18], numerical inversion of the Laplace transform [29], to name just a few. Chebyshev polynomials in particular are a practical choice, since they feature fast algorithms based on the FFT [37]. These properties have enabled the Chebfun project [26], for example. General spectral expansions in terms of Jacobi polynomials offer spectral convergence: faster than algebraic convergence for infinitely differentiable functions, geometric convergence for functions analytic in a neighborhood of the expansion interval and even faster convergence for entire functions. Due to these benefits, spectral methods using orthogonal polynomials have been the methods of choice for calculating high accuracy solutions in a broad range of applications (see, for example, [6, 8, 19, 21, 31, 35, 37]).

The objectives of this paper are two-fold, namely to describe algorithms for

1. the *fast* computation of Jacobi expansion coefficients of analytic functions,
2. and the *accurate* computation of those coefficients.

In general one has to choose between maximal speed and maximal accuracy with our algorithms. However, for wide classes of functions, including meromorphic functions, these two objectives can also be reached simultaneously. This observation motivates their combination in a single paper. It should be noted that in any case the fast methods are always accurate with respect to absolute errors of the coefficients. Thus, the difference lies only with the coefficients that are very small.

The contents of this paper have been inspired mainly by a fast method for the computation of Legendre coefficients due to Iserles [24] and an accurate method for the computation of high-order derivatives in the complex plane due to Bornemann [5]. To be more precise, first we adapt the analysis of [5] to the computation of Chebyshev coefficients of the first and second kinds and we demonstrate that they can be computed with small relative error, in many cases on the order of the machine precision. Next, we generalize the computational scheme of [24] to Jacobi polynomials and we provide a new analysis. Before presenting our results, we elaborate briefly on the above references and on other existing research in this area.

1.1 Fast methods for computing polynomial expansions

Several methods have been described for the fast computation of polynomial expansion coefficients [2, 12, 11, 14, 13, 33, 22, 25, 24, 9, 7, 38]. In particular, the special case of Legendre polynomials has received the most study [2, 11, 22, 24, 9, 38]. A popular strategy is to use the FFT, with computations based on function evaluations at the Chebyshev points [2, 12, 11, 33]. More general sets of evaluation points have been treated using Fast

Multipole Methods [14], using a particular matrix-factorization of the problem stated as a matrix-vector product [13], using non-uniform FFT's [25] and using numerical computation of Abel transforms [9]. All these methods exhibit $\mathcal{O}(N \log N)$ computational complexity, possibly with additional logarithmic factors, for the computation of the first N coefficients. The accuracy is sometimes restricted to a chosen small value ϵ. Scaling ϵ with N in a particular way, so that larger values of N yield higher accuracy, may affect the stated computational complexities of the methods.

Methods based on function evaluations in the Chebyshev points are, at least mathematically, equivalent to an expansion in Chebyshev polynomials of the first kind. The coefficients of this expansion can then be rearranged in varying ways in order to form the Legendre expansion or other expansions. A unique feature of the fast methods for Legendre polynomials in [24] and more general ultraspherical polynomials in [7] is that the evaluation points may be in the complex plane, if the function to be approximated is analytic. We will show further on that this approach is also implicitly equivalent to expanding in a set of Chebyshev polynomials (of the second kind, in this case), and then rearranging the coefficients. In the current paper, we make these two steps explicit and in the process we generalize the approach of [24, 7] to Jacobi polynomials. Furthermore, we derive efficient and general recurrence relations that enable the transformation from one polynomial basis to another.

1.2 Accurate computation of high-order derivatives

Computing derivatives of a function numerically is a notoriously ill-conditioned problem, especially for high-order derivatives [28]. It was shown by Bornemann in [5] that computation of high-order derivatives through Cauchy integrals in the complex plane is, in fact, stable. To be precise, consider the power series of a function analytic at the origin, with radius of convergence R,

$$f(z) = \sum_{k=0}^{\infty} t_k z^k, \quad |z| < R.$$

The coefficients t_n can be written as a contour integral along a disc with radius $r < R$,

$$t_n = \frac{f^{(n)}(0)}{n!} = \frac{1}{2\pi i} \int_{|z|=r} \frac{f(z)}{z^{n+1}} \mathrm{d}z. \tag{1.1}$$

Such integrals can be evaluated quickly with the FFT for a range of n with the parametrization $z = re^{i\theta}$. However, Bornemann showed that for each n an optimal value of r exists, such that evaluating the contour integral is, for most analytic functions, perfectly stable. A detailed analysis is given in [5] to characterize the optimal radius, exactly or approximately, for several classes of analytic functions. Using the optimal radius r for each value of n precludes the use of the FFT. However, small *relative error* of the coefficient t_n is guaranteed. As a result, for most analytic functions t_n can be computed with a number of digits close to the maximal accuracy allowed by the machine precision and with values of n ranging up to millions.

1.3 Main results and outline of this paper

We describe and analyze an efficient way to compute Jacobi expansions by first computing an expansion in Chebyshev polynomials, of the first or of the second kind, and then rearranging the coefficients. There is no clear advantage to either of the two kinds.

The first step, the computation of the Chebyshev coefficients, is performed in the complex plane. We use the trapezoidal rule for the integrals

$$a_n = \frac{1}{\pi\rho^n}\int_0^{2\pi} f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) e^{-in\theta} d\theta \tag{1.2}$$

and

$$b_n = \frac{1}{2\pi\rho^n}\int_0^{2\pi} f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)(1-(\rho e^{i\theta})^{-2}) e^{-in\theta} d\theta. \tag{1.3}$$

The latter integrals (for b_n) are those appearing in [24, (3.5)] and in [7, (3.2)]. We show in §2 that the values a_n and b_n correspond to coefficients of polynomial expansions using Chebyshev polynomials of the first and second kind respectively. The value of $\rho \geq 1$ is arbitrary and limited by the analyticity of f.

We show in §3 that the trapezoidal rule for these integrals is always stable with respect to absolute errors of the normalized values $\rho^n a_n$ and $\rho^n b_n$. Furthermore, we show that in many cases for each n an optimal value $\rho^*(n)$ exists, such that the computation is stable with respect to relative errors. This implies that also very small coefficients can be computed to high accuracy. The cases depend on the properties of f in the complex plane and they correspond to the cases described by Bornemann in [5] in the context of computing high-order derivatives. The integrals (1.2) and (1.3) play the role of the Cauchy integral (1.1) in [5].

We rearrange the Chebyshev expansions into a Jacobi expansion in §4. The connection coefficients that appear in this process are analysed in §5. In particular, we derive explicit and stable recurrence relations for these coefficients and we perform an asymptotic analysis of the coefficients, in order to prove stability results for the Jacobi expansions later on.

We formulate the results thus far in an algorithmic form using the FFT in §6. This is the approach that maximizes computational efficiency and it corresponds to choosing the same value of ρ for all coefficients. The theory is illustrated with numerical examples demonstrating efficiency in §7.

Finally, we describe the approach that maximizes accuracy for Chebyshev and more general Jacobi expansions in §8, by choosing ρ dependent on n for each coefficient. Numerical examples demonstrate the theory in §9. We show that repeated differentiation of the polynomial expansions can be performed without loss of precision in §10.

2 Chebyshev expansion coefficients

Chebyshev expansions are widely used in numerical analysis. It is well known that the Chebyshev coefficients can be computed efficiently by the FFT and that this computation is numerically stable with respect to absolute errors. In the following, we will show that this strategy remains stable when performing computations along certain contours in the complex plane. For the stability with respect to relative errors, a different theory should be considered. We begin our analysis with an alternative integral expression of Chebyshev coefficients.

2.1 Chebyshev expansion of the first kind

Let $T_n(x)$ denote the Chebyshev polynomial of the first kind of degree n, as defined by

$$T_n(\cos\theta) = \cos(n\theta), \quad n \geq 0.$$

If a function $f(x)$ satisfies a Dini-Lipschitz condition on the interval $[-1, 1]$ then it can be expanded uniformly in terms of $T_n(x)$ as [27, Thm. 5.7]

$$f(x) = \sum_{n=0}^{\infty}{}' a_n T_n(x), \tag{2.1}$$

where the prime indicates that the first term of the sum should be halved and the coefficients are given by the integrals

$$a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)T_n(x)}{\sqrt{1-x^2}} dx, \quad n \geq 0. \tag{2.2}$$

We are interested in integral expressions for a_n in the complex plane. Let $\mathcal{E}_\rho$ denote the *Bernstein ellipse* in the complex plane

$$\mathcal{E}_\rho = \left\{ z \in \mathbb{C} \;\middle|\; z = \frac{1}{2}\big(\rho e^{i\theta} + \rho^{-1}e^{-i\theta}\big), \;\; 0 \leq \theta \leq 2\pi \right\}.$$

We will always assume $\rho \geq 1$. We denote the interior of this ellipse by

$$\mathcal{D}_\rho = \left\{ z \in \mathbb{C} \;\middle|\; z = \frac{1}{2}\big(re^{i\theta} + r^{-1}e^{-i\theta}\big), \;\; 1 \leq r < \rho, \; 0 \leq \theta \leq 2\pi \right\}.$$

It is well known that the Bernstein ellipses have foci ± 1 and their major and minor semiaxis lengths summing to ρ. In the following, we will often use the notation

$$z(u) = \frac{1}{2}(u + u^{-1}), \tag{2.3}$$

where typically $u = \rho e^{i\theta}$ is a point on the circle with radius ρ and $z(u)$ lies on the Bernstein ellipse $\mathcal{E}_\rho$. The inverse expression (the one that satisfies $|u| > 1$) is

$$u(z) = z + \sqrt{z^2 - 1}. \tag{2.4}$$

The following integral expression for a_n was derived by Elliott in [15, Eqn. (28)] for entire functions $f(z)$ by using Cauchy's integral formula. Here, we shall give a simpler proof based on Laurent series expansions. We further show that the expression remains valid for functions analytic only in a neighborhood of the interval $[-1, 1]$.

Lemma 2.1. *If f is analytic inside and on the Bernstein ellipse $\mathcal{E}_\rho$ with $\rho > 1$, then for each $n \geq 0$ we have*

$$a_n = \frac{1}{\pi \rho^n} \int_0^{2\pi} f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) e^{-in\theta} d\theta. \tag{2.5}$$

Proof. First we recall that the Chebyshev expansion is convergent in the interior of the greatest ellipse in which $f(x)$ is analytic [36, Thm. 9.1.1]. Moreover, recall the definition of the Chebyshev polynomials of the first kind in the complex plane [27, Eqn. (1.47)]

$$T_k(z(u)) = \frac{1}{2}(u^k + u^{-k}), \tag{2.6}$$

which implies

$$\begin{aligned} f(z(u)) &= \sum_{n=0}^{\infty}{}' a_n T_n(z(u)) \\ &= \frac{1}{2} \sum_{n=-\infty}^{\infty} a_{|n|} u^n, \end{aligned}$$

where $z(u)$ is inside or on the boundary of $\mathcal{E}_\rho$. For each $n \geq 0$, the last equality shows that the n-th Chebyshev coefficient of $f(x)$ corresponds exactly the n-th coefficient of the Laurent series expansion of $2f(z(u))$ at the origin. Therefore, we can deduce immediately that for each $n \geq 0$,

$$\begin{aligned} a_n &= \frac{1}{2\pi i} \oint_{\mathcal{C}_\rho} 2 f(z(u)) u^{-n-1} du \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} f(z(u)) u^{-n-1} du. \end{aligned}$$

where $\mathcal{C}_\rho$ denotes the circle $|u| = \rho$. Substituting $u = \rho e^{i\theta}$ into the last equality yields the desired result. $\square$

We make some further comments regarding (2.2) and (2.5):

- We define the *normalized* Chebyshev coefficient to be $\rho^n a_n$. In spite of its dependence on the parameter ρ, this definition is a natural one because the FFT-based algorithms presented further on yield a small absolute error of the normalized coefficients for a given value of ρ.
- Letting $\rho \to 1$ and using the change of variable $x = \cos\theta$, (2.5) reduces to (2.2).
- In the same limit $\rho \to 1$, we also obtain the well known expression

  $$a_n = \frac{1}{\pi} \int_0^{2\pi} f(\cos\theta) e^{-in\theta} d\theta = \frac{1}{\pi} \int_0^{2\pi} f(\cos\theta) \cos(n\theta) d\theta. \tag{2.7}$$

  The last expression is often the starting point for introducing fast algorithms based on the discrete cosine or Fourier transform to evaluate the Chebyshev coefficients (see, for example, [37, 17, 23, 27]).

- Integral expressions for a_n in the complex plane date back at least to Bernstein [4]. They have been used, among other purposes, to estimate the decay rates of Chebyshev coefficients (see, for example, [15, 34]). To the best of our knowledge, they have not been used for computational purposes. One obvious reason is that it is not clear whether there is any advantage in evaluating (2.5) compared to evaluating (2.7), especially in view of the existence of simple, fast and stable algorithms for the latter. Furthermore, expression (2.5) requires analyticity of f. We will show later on that expression (2.5) can be used to give better approximations in the sense that the relative error of each Chebyshev coefficient can be minimized by choosing an optimal value of ρ.

- For example, (2.5) leads to the well-known bound [34, Thm. 3.8]

$$|a_n| \leq \frac{2\mathcal{M}}{\rho^n},$$

where $\mathcal{M}$ is the maximum absolute value of f along the Berstein ellipse $\mathcal{E}_\rho$.

2.2 Chebyshev expansion of the second kind

Let $U_n(x)$ denote the Chebyshev polynomial of the second kind of degree n, defined by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad n \geq 0.$$

The Chebyshev expansion of the second kind is given by

$$f(x) = \sum_{n=0}^{\infty} b_n U_n(x), \tag{2.8}$$

where

$$b_n = \frac{2}{\pi}\int_{-1}^{1} \sqrt{1-x^2} f(x) U_n(x) dx. \tag{2.9}$$

Lemma 2.2. *If f is analytic inside and on the Bernstein ellipse $\mathcal{E}_\rho$ with $\rho > 1$, then for each $n \geq 0$ we have*

$$b_n = \frac{1}{2\pi\rho^n}\int_0^{2\pi} f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)(1-(\rho e^{i\theta})^{-2}) e^{-in\theta} d\theta. \tag{2.10}$$

Proof. Using the definition of the Chebyshev polynomials of the second kind in the complex plane [27, Eqn. (1.51)]

$$U_k(z(u)) = \frac{u^{k+1} - u^{-k-1}}{u - u^{-1}},$$

we have that

$$
\begin{aligned}
f(z(u)) &= \sum_{n=0}^{\infty} b_n U_n(z(u)) \\
&= \sum_{n=0}^{\infty} b_n \frac{u^{n+1} - u^{-n-1}}{u - u^{-1}}.
\end{aligned}
$$

Multiplying both sides of the last equality by $1 - u^{-2}$ gives

$$
f(z(u))(1 - u^{-2}) = \sum_{n=0}^{\infty} b_n (u^n - u^{-n-2}).
$$

For each $n \geq 0$, the above equality shows that b_n corresponds exactly to the n-th coefficient of the Laurent series expansion of $f(z(u))(1 - u^{-2})$ at the origin. Therefore, we can deduce immediately that for each $n \geq 0$,

$$
b_n = \frac{1}{2\pi i} \oint_{\mathcal{C}_\rho} f(z(u))(1 - u^{-2}) u^{-n-1} du. \tag{2.11}
$$

Substituting $u = \rho e^{i\theta}$ into the last equality yields the desired result. $\square$

Here, too, we will make some further comments regarding (2.10):

- Similarly as before, we define the *normalized* Chebyshev coefficient to be $\rho^n b_n$.
- Letting $\rho \to 1$ in (2.10) yields,

$$
\begin{aligned}
b_n &= \frac{1}{2\pi} \int_0^{2\pi} f(\cos\theta)(1 - e^{-2i\theta}) e^{-in\theta} d\theta \\
&= \frac{1}{\pi} \int_0^{2\pi} f(\cos\theta) \sin\theta \sin(n+1)\theta d\theta \\
&= \frac{2}{\pi} \int_{-1}^{1} \sqrt{1 - x^2} f(x) U_n(x) dx, \qquad (2.12)
\end{aligned}
$$

  which corresponds to (2.9).

- Expression (2.11) can be further written as

$$
\begin{aligned}
b_n &= \frac{1}{2\pi i} \oint_{\mathcal{C}_\rho} f(z(u))(1 - u^{-2}) u^{-n-1} du \\
&= \frac{1}{\pi i} \oint_{\mathcal{E}_\rho} f(z(u)) u(z)^{-n-1} dz(u),
\end{aligned}
$$

  which can be used to established the rate of decay of the coefficients b_n (see Eqn. (4.10) below).

- From the inspection of the formulas (2.5) and (2.10), it is clear that a_n and b_n are related for all ρ by

$$
b_n = \frac{a_n - a_{n+2}}{2}. \tag{2.13}
$$

3 Absolute and relative stability

From (2.5) and (2.10) we see that both kinds of Chebyshev coefficients can be expressed in terms of contour integrals with integrands that are periodic functions of θ. Thus, these coefficients can be approximated efficiently by applying the trapezoidal rule. In the following we shall consider stability of the computation of the Chebyshev coefficients with respect to absolute and relative errors of the normalized coefficients, respectively.

3.1 Absolute stability

For the Chebyshev coefficients of the first kind, using an m-point trapezoidal rule yields

$$a_n(m,\rho) = \frac{2}{m\rho^n} \sum_{j=0}^{m-1} f\left(\tfrac{1}{2}(\rho e^{2\pi ij/m} + \rho^{-1} e^{-2\pi ij/m})\right) e^{-2\pi ijn/m}. \tag{3.1}$$

Let $\mathcal{P}_m$ be the set of all polynomials of degree $\leq m$ and let

$$\|f - s\|_{\mathcal{D}_\rho} := \max_{z\in\overline{\mathcal{D}}_\rho} |f(z) - s(z)|.$$

Note that by the maximum modulus principle we have the equality of norms

$$\|f - s\|_{\mathcal{D}_\rho} = \|f - s\|_{\mathcal{E}_\rho} := \max_{z\in\mathcal{E}_\rho} |f(z) - s(z)|,$$

so that from now on we simply use $\|\cdot\|_{\mathcal{E}_\rho}$.

Furthermore, let

$$s_m(z) = {\sum_{k=0}^{m-1}}' \eta_k T_k(z)$$

denote the best $(m-1)$-th degree polynomial approximation to $f(z)$ on and inside the ellipse $\mathcal{E}_\rho$, i.e.,

$$\|f(z) - s_m(z)\|_{\mathcal{E}_\rho} := \inf_{s\in\mathcal{P}_{m-1}} \|f(z) - s(z)\|_{\mathcal{E}_\rho}.$$

In the following, we will always assume that the *sampling condition* $m > n$ holds, in order to avoid aliasing of the complex exponentials in (3.1). We refer the reader to [5, §2.1] for a discussion and justification of this condition.

Theorem 3.1. *For $1 \leq n < m$, we have the following error estimate*

$$|a_n - a_n(m,\rho)| \leq \frac{4}{\rho^n} \|f - s_m\|_{\mathcal{E}_\rho} + \frac{|\eta_{m-n}|}{\rho^m}, \tag{3.2}$$

and for $n = 0$,

$$|a_0 - a_0(m,\rho)| \leq 4\|f - s_m\|_{\mathcal{E}_\rho}. \tag{3.3}$$

Proof. Let $z(\rho,\theta)=\frac{1}{2}(\rho e^{i\theta}+(\rho e^{i\theta})^{-1})$. From (2.5) and (3.1), we have

$$\begin{aligned}
a_n - a_n(m,\rho) &= \frac{1}{\pi\rho^n}\int_0^{2\pi} f\left(z(\rho,\theta)\right)e^{-in\theta}d\theta - \frac{2}{m\rho^n}\sum_{j=0}^{m-1} f(z(\rho,2\pi j/m))e^{-2\pi ijn/m} \\
&= \frac{1}{\pi\rho^n}\int_0^{2\pi}[f\left(z(\rho,\theta)\right) - s_m\left(z(\rho,\theta)\right)]e^{-in\theta}d\theta \\
&\quad + \left(\frac{1}{\pi\rho^n}\int_0^{2\pi} s_m\left(z(\rho,\theta)\right)e^{-in\theta}d\theta - \frac{2}{m\rho^n}\sum_{j=0}^{m-1} s_m(z(\rho,2\pi j/m))e^{-2\pi ijn/m}\right) \\
&\quad + \frac{2}{m\rho^n}\sum_{j=0}^{m-1}[s_m(z(\rho,2\pi j/m)) - f(z(\rho,2\pi j/m))]e^{-2\pi ijn/m}.
\end{aligned}$$

We use E_1 to denote the first integral of the last equality, E_2 denotes the difference contained in the brackets and E_3 denotes the remaining part. Explicit estimates can be established for E_1 and E_3,

$$|E_1| \le \frac{2}{\rho^n}\|f-s_m\|_{\mathcal{E}_\rho}, \quad |E_3| \le \frac{2}{\rho^n}\|f-s_m\|_{\mathcal{E}_\rho}.$$

For E_2, using (2.6) we have

$$\begin{aligned}
E_2 &= \frac{1}{\pi\rho^n}\int_0^{2\pi} s_m\left(z(\rho,\theta)\right)e^{-in\theta}d\theta - \frac{2}{m\rho^n}\sum_{j=0}^{m-1} s_m(z(\rho,2\pi j/m))e^{-2\pi ijn/m} \\
&= \eta_n - \frac{1}{m\rho^n}\sum_{k=-(m-1)}^{m-1}\eta_{|k|}\rho^k\left(\sum_{j=0}^{m-1} e^{2\pi ij(k-n)/m}\right) \\
&= \begin{cases} 0, & n=0, \\ -\frac{\eta_{m-n}}{\rho^m}, & 1\le n<m. \end{cases}
\end{aligned}$$

Combining this with estimates of E_1 and E_3 gives the desired results. □

From Theorem 3.1 we can see that if f is a polynomial of degree n, then we have $s_m=f$ if $m\ge n+1$. This implies that the trapezoidal rule (3.1) computes the k-th Chebyshev coefficient of f exactly if $m\ge k+n+1$ since $\eta_{m-n}=0$. Thus, if we choose $m\ge 2n+1$, then all Chebyshev coefficients of the polynomial function f can be computed exactly by the trapezoidal rule (3.1).

Theorem 3.1 implies for any function f that the difference in the normalized coefficients $\rho^n a_n - \rho^n a_n(m,\rho)$ is on the order of ϵ, if m is sufficiently large so that η_{m-n} is small. This assertion is true, since from

$$\begin{aligned}
|\eta_k - a_k| &= \left|\frac{1}{\pi i}\oint_{\mathcal{C}_\rho}(s_m(z(u)) - f(z(u)))u^{-n-1}du\right| \\
&\le \frac{2}{\rho^k}\|f(z)-s_m(z)\|_{\mathcal{E}_\rho},
\end{aligned}$$

it follows that

$$
\begin{aligned}
|\eta_k| &\le |a_k| + \frac{2}{\rho^k}\|f(z) - s_m(z)\|_{\mathcal{E}_\rho} \\
&\le \frac{2}{\rho^k}(\mathcal{M} + \|f(z) - s_m(z)\|_{\mathcal{E}_\rho}).
\end{aligned}
$$

This estimate implies that the coefficients η_k decay exponentially fast.

Similarly, for the Chebyshev coefficients b_n, the m-point trapezoidal rule gives

$$
b_n(m,\rho) = \frac{1}{m\rho^n}\sum_{j=0}^{m-1} f\left(z(\rho, 2\pi j/m)\right)(1-\rho^{-2}e^{-4\pi i j/m})e^{-2\pi i j n/m}. \tag{3.4}
$$

Theorem 3.2. *We have the following error estimate*

$$
|b_n - b_n(m,\rho)| \le \frac{2(1-\rho^{-2})}{\rho^n}\|f - s_m\|_{\mathcal{E}_\rho} + \begin{cases} \frac{|\eta_{m-2}|}{2\rho^m}, & n = 0, \\ \frac{|\eta_{m-n} - \eta_{m-n-2}|}{2\rho^m}, & n = 1,\dots,m-3, \\ \frac{|\eta_{m-n} - \eta_{n+2-m}|}{2\rho^m}, & n = m-2, m-1\ . \end{cases} \tag{3.5}
$$

Proof. The proof is essentially the same as that of Theorem 3.1. We omit the details. □

Similarly to (3.1), if f is a polynomial of degree n, then b_k is computed exactly by the trapezoidal rule (3.4) if $m \ge k+n+3$. This implies that all $\{b_k\}_{k=0}^n$ are computed exactly by the trapezoidal rule (3.4) if we choose $m \ge 2n+3$.

Suppose now that $\hat{f}$ is a perturbation of f and

$$
\|\hat{f}(z) - f(z)\|_{\mathcal{E}_\rho} \le \epsilon.
$$

The perturbed Chebyshev coefficients are given by

$$
\hat{a}_n = \frac{1}{\pi\rho^n}\int_0^{2\pi} \hat{f}\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)e^{-in\theta}d\theta. \tag{3.6}
$$

Meanwhile, the computed Chebyshev coefficients are given by

$$
\hat{a}_n(m,\rho) = \frac{2}{m\rho^n}\sum_{j=0}^{m-1}\hat{f}\left(\tfrac{1}{2}(\rho e^{2\pi i j/m} + \rho^{-1}e^{-2\pi i j/m})\right)e^{-2\pi i j n/m}. \tag{3.7}
$$

A simple bound can be derived for the Chebyshev coefficients of the first kind

$$
|a_n - \hat{a}_n| \le \frac{2\epsilon}{\rho^n}, \quad |\hat{a}_n(m,\rho) - a_n(m,\rho)| \le \frac{2\epsilon}{\rho^n}. \tag{3.8}
$$

Then the following estimate also holds

$$
\begin{aligned}
\rho^n|\hat{a}_n(m,\rho) - a_n| &\le \rho^n|a_n(m,\rho) - \hat{a}_n(m,\rho)| + \rho^n|a_n - a_n(m,\rho)| \\
&\le 2\epsilon + \begin{cases} 4\|f - s_m\|_{\mathcal{E}_\rho}, & n = 0, \\ 4\|f - s_m\|_{\mathcal{E}_\rho} + \frac{|\eta_{m-n}|}{\rho^{m-n}}, & 1 \le n < m. \end{cases}
\end{aligned}
$$

A similar estimate can be established for the coefficients of the second kind b_n.

We conclude that the trapezoidal rule for the Chebyshev coefficients is numerically stable with respect to the absolute error of the normalized coefficients. If we only consider this absolute stability, then it is sufficient to choose the same ρ simultaneously for all Chebyshev coefficients and to compute these coefficients with the same trapezoidal rule. Furthermore, from (3.1) we see that the sum on the right hand side is perfectly suitable to utilize the FFT. Thus, the first N Chebyshev coefficients can be efficiently evaluated with a single FFT in $\mathcal{O}(N \log N)$ operations.

3.2 Relative stability

If we consider the relative error of the computed coefficients, computing all Chebyshev coefficients with a single ρ is not optimal. A comprehensive analysis of the relative stability of computing the Taylor expansion coefficients of analytic functions from contour integrals along circles in the complex plane has been given by Bornemann in [5]. Here we extend his analysis to the current setting of Chebyshev coefficients.

Suppose $\hat{f}$ is a perturbation of f with the form

$$\hat{f}(z) = f(z)(1 + \epsilon_\rho(z)), \quad |\epsilon_\rho(z)| \leq \epsilon.$$

There is a simple upper bound on the error of the perturbed Chebyshev coefficients,

$$\begin{aligned} |a_n - \hat{a}_n| &= \frac{1}{\pi \rho^n} \left| \int_0^{2\pi} f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) \epsilon_\rho \left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) e^{-in\theta} d\theta \right| \\ &\leq \frac{\epsilon}{\pi \rho^n} \int_0^{2\pi} \left| f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) \right| d\theta, \end{aligned}$$

which leads to

$$\frac{|a_n - \hat{a}_n|}{|a_n|} \leq \kappa^{\mathrm{Ch1}}(n, \rho)\epsilon, \tag{3.9}$$

where the quantity

$$\kappa^{\mathrm{Ch1}}(n, \rho) = \frac{\int_0^{2\pi} \left| f\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) \right| d\theta}{\left| \int_0^{2\pi} f\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) e^{-in\theta} d\theta \right|} \geq 1, \tag{3.10}$$

is called the condition number of the integral. Similarly, for the Chebyshev coefficients of the second kind, we have

$$\frac{|b_n - \hat{b}_n|}{|b_n|} \leq \kappa^{\mathrm{Ch2}}(n, \rho)\epsilon, \tag{3.11}$$

with the corresponding condition number given by

$$\kappa^{\mathrm{Ch2}}(n, \rho) = \frac{\int_0^{2\pi} \left| f\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) (1 - (\rho e^{i\theta})^{-2}) \right| d\theta}{\left| \int_0^{2\pi} f\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right) (1 - (\rho e^{i\theta})^{-2}) e^{-in\theta} d\theta \right|}. \tag{3.12}$$

3.3 Condition number of the contour integrals

We consider the condition number of the integral expressions for the Chebyshev coefficients of the first kind. The corresponding integrals for the Chebyshev coefficients of the second kind can be analyzed similarly.

We first rewrite the condition number as

$$\kappa^{\mathrm{Ch1}}(n,\rho) = \frac{M(\rho)}{|a_n|\rho^n}, \tag{3.13}$$

where

$$M(\rho) = \frac{1}{\pi}\int_0^{2\pi} \left| f\left(\tfrac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)\right| d\theta. \tag{3.14}$$

Note that $M(\rho) = M(\rho^{-1})$.

We proceed by analyzing this function $M(\rho)$. It is the analogue of the function

$$M_1(r) = \frac{1}{2\pi}\int_0^{2\pi} |f(re^{i\theta})| d\theta, \tag{3.15}$$

which appears in the condition number for the Cauchy integral (1.1) in the analysis of Bornemann. He showed that $M_1(r)$ has a unique minimum at a finite value of r. The starting point of this analysis is a theorem on the growth of $M_1(r)$ [5, Thm 4.1] originally due to Hardy in 1915 [20]. Unfortunately, Hardy's original proof for $M_1(r)$ does not apply for the analysis of the function $M(\rho)$, since the integrand of (3.14) is not analytic at the origin. In the following theorem we formulate the corresponding result for $M(\rho)$, with a method of proof that still largely follows that of Hardy.

Theorem 3.3. *Let f be analytic in any ellipse $\mathcal{E}_\rho$ with $1 \le \rho < R$. The function $M(\rho)$ satisfies the following properties:*

1. *$M(\rho)$ is continuously differentiable.*
2. *If f is not a constant, $M(\rho)$ is strictly increasing as ρ grows.*
3. *If $f \not\equiv 0$, then $\log M(\rho)$ is a convex function of $\log\rho$.*

Proof. Our proof closely follows the ideas of [20]. We will first consider the case where f has no zero inside the ellipse R. Let $u = \rho e^{i\theta}$ and $F(u) = f(\frac{1}{2}(u + u^{-1}))$ and define their corresponding logarithms as

$$\log u = y + i\theta, \qquad \log F(u) = \Xi + i\Phi.$$

It follows that Ξ and Φ are harmonic conjugate functions of y and θ. Let $\varphi(z)$ be a real function of Ξ and Φ with continuous second order derivatives. According to [20, Eqn. A], we have

$$\frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial\theta^2} = \left(\frac{\partial^2\varphi}{\partial\Xi^2} + \frac{\partial^2\varphi}{\partial\Phi^2}\right) H^2, \tag{3.16}$$

where

$$H^2 = \left(\frac{\partial \Xi}{\partial y}\right)^2 + \left(\frac{\partial \Phi}{\partial y}\right)^2. \tag{3.17}$$

With the choice $\varphi(\Xi) = e^{\Xi}$ the function $M(\rho)$ under consideration can be written as

$$M(\rho) = \frac{1}{\pi}\int_0^{2\pi} \varphi(\Xi) d\theta.$$

For convenience, in the following we denote the function $M(\rho)$ by a new function $\psi(y)$. Using the Cauchy-Schwarz inequality and (3.17), we obtain

$$\begin{aligned}
|\psi'(y)|^2 &= \frac{1}{\pi^2}\left(\int_0^{2\pi} \varphi(\Xi)\frac{\partial \Xi}{\partial y} d\theta\right)^2 \\
&\leq \frac{1}{\pi^2}\int_0^{2\pi} \varphi(\Xi) d\theta \int_0^{2\pi} \varphi(\Xi)\left(\frac{\partial \Xi}{\partial y}\right)^2 d\theta \\
&= \frac{\psi(y)}{\pi}\int_0^{2\pi} \varphi(\Xi)\left(\frac{\partial \Xi}{\partial y}\right)^2 d\theta \\
&\leq \frac{\psi(y)}{\pi}\int_0^{2\pi} \varphi(\Xi) H^2 d\theta. \qquad (3.18)
\end{aligned}$$

On the other hand, using (3.16), we have

$$\begin{aligned}
\psi''(y) &= \frac{1}{\pi}\int_0^{2\pi} \frac{\partial^2 \varphi}{\partial y^2} d\theta \\
&= \frac{1}{\pi}\int_0^{2\pi} \frac{\partial^2 \varphi}{\partial \Xi^2} H^2 d\theta - \frac{1}{\pi}\int_0^{2\pi} \frac{\partial^2 \varphi}{\partial \theta^2} d\theta \\
&= \frac{1}{\pi}\int_0^{2\pi} \varphi(\Xi) H^2 d\theta, \qquad (3.19)
\end{aligned}$$

where in the second step we have used the fact that $\varphi(\Xi)$ is a periodic function of θ. Consequently, $\psi''(y) \geq 0$ and we can easily deduce that $\psi'(y)$ is increasing as y grows. Moreover, note that $\psi(y)$ is even and this implies $\psi'(0) = 0$. Hence, $\psi'(y) \geq 0$ for $y \geq 0$ and the second assertion follows. For the third assertion, from (3.19) and (3.18), we have

$$\psi(y)\psi''(y) \geq |\psi'(y)|^2.$$

Hence, $\log \psi(y)$ is a convex function of y and the third assertion holds.

Next, we consider the case where $f(x)$ does have zeros inside the ellipse. More specifically, suppose that

$$f(x) = (x - x_0)^m f_1(x), \tag{3.20}$$

where $m > 0$, $x_0 = \frac{1}{2}(u_0 + u_0^{-1})$ and $u_0 = re^{i\phi}$ with $1 < r < R$ and R is the largest radius of the ellipse. Furthermore, like Hardy, we assume for simplicity of presentation that $f_1(\frac{1}{2}(u + u^{-1}))$ has no zero throughout an interval $r - \epsilon \leq \rho \leq r + \epsilon$ for $\epsilon > 0$

sufficiently small. We now intend to show that the derivative of $M(\rho)$ is uniformly continuous throughout the aformentioned interval of ρ. Let $u = \rho e^{i\theta} = \xi + i\eta$ and $F(u) = f(\frac{1}{2}(u+u^{-1})) = \chi + i\upsilon$. For any real continuous function ψ of χ and υ, using [20, Eqn. B], we have

$$\left(\frac{\partial\psi}{\partial\xi}\right)^2 + \left(\frac{\partial\psi}{\partial\eta}\right)^2 = \left\{\left(\frac{\partial\psi}{\partial\chi}\right)^2 + \left(\frac{\partial\psi}{\partial\upsilon}\right)^2\right\}\left|\frac{dF}{du}\right|^2,$$

In particular, taking $\psi(\chi,\upsilon) = |F(u)| = \sqrt{\chi^2+\upsilon^2}$ yields

$$\left(\frac{\partial\psi}{\partial\xi}\right)^2 + \left(\frac{\partial\psi}{\partial\eta}\right)^2 = \left|\frac{dF}{du}\right|^2.$$

On the other hand,

$$\left|\frac{\partial\psi}{\partial\rho}\right| = \left|\frac{\partial\psi}{\partial\xi}\cos\theta + \frac{\partial\psi}{\partial\eta}\sin\theta\right| \le \sqrt{\left(\frac{\partial\psi}{\partial\xi}\right)^2 + \left(\frac{\partial\psi}{\partial\eta}\right)^2} = \left|\frac{dF}{du}\right|.$$

Since

$$\begin{aligned}\frac{dF}{du} = \frac{1}{2}(1-u^{-2})\Bigg[&\frac{m}{2^{m-1}}(u-u_0)^{m-1}\left(1-\frac{1}{uu_0}\right)^{m-1} f_1\left(\frac{1}{2}(u+u^{-1})\right)\\ &+\frac{1}{2^m}(u-u_0)^m\left(1-\frac{1}{uu_0}\right)^m f_1'\left(\frac{1}{2}(u+u^{-1})\right)\Bigg],\end{aligned}$$

it follows that

$$\left|\frac{dF}{du}\right| \le K|u-u_0|^{m-1},$$

where K is a constant. Thus,

$$\left|\frac{\partial M}{\partial\rho}\right| \le \frac{1}{\pi}\int_0^{2\pi}\left|\frac{\partial\psi}{\partial\rho}\right|d\theta \le \frac{1}{\pi}\int_0^{2\pi}\left|\frac{dF}{du}\right|d\theta \le \frac{K}{\pi}\int_0^{2\pi}|u-u_0|^{m-1}d\theta.$$

Following the proof of Hardy [20, p. 275], the last integral on the right hand side of the above equation is uniformly convergent. This completes the proof.

□

Since $\log\kappa^{\mathrm{Ch1}}(n,\rho) = \log M(\rho) - \log|a_n| - n\log\rho$, we have the following corollary.

Corollary 3.4. *Let f be analytic on and inside an ellipse $\mathcal{E}_\rho$ with $1 \le \rho < R$. Then for each Chebyshev coefficient $a_n \ne 0$, we have*

1. *$\kappa^{\mathrm{Ch1}}(n,\rho)$ is continuously differentiable with respect to ρ.*
2. *If f is not a constant, $\log(\kappa^{\mathrm{Ch1}}(n,\rho))$ is a convex function of $\log\rho$.*

In the analysis of Bornemann, [5, Theorem 4.1] and [5, Corollary 4.2] are the key steps in proving that an optimal radius exists for Cauchy integrals of the form (1.1). Afterwards, it remains to analyze the limits $r \to 0$ and $r \to \infty$. The limit $r \to 0$ is always unstable. The limit in the other direction depends on the analyticity properties of f in the complex plane.

With our analogous Theorem 3.3 and Corollary 3.4 at hand, we can reuse Bornemann's results in the context of Chebyshev coefficients with only slight adjustments. One major difference concerns the difference between the limits for small ρ and r. Indeed, contrary to the limit $r \to 0$ in the setting of Taylor series coefficients, there is no numerical instability associated with the limit $\rho \to 1$. Recall also that $M(\rho) = M(\rho^{-1})$, so that we don't consider the case $\rho < 1$. It is clear that $M(\rho)$ is bounded as $\rho \to 1$ and we have:

Theorem 3.5. *Assume f is analytic in any ellipse $\mathcal{E}_\rho$ with $1 \le \rho < R$ and let a_n be nonzero. Then*

$$\lim_{\rho \to 1} \kappa^{\mathrm{Ch1}}(n, \rho) = \frac{1}{\pi |a_n|} \int_0^{2\pi} |f(\cos\theta)| d\theta.$$

Proof. This follows from the definitions (3.13) and (3.14). □

Two interesting results to formulate explicitly are as follows.

Theorem 3.6. *Assume f is an entire transcendental function and*

$$M(\rho) \sim e^{\mu \rho^\nu} \rho^\varsigma, \quad \rho \to \infty, \tag{3.21}$$

where μ is positive and finite and ν is positive. Then the asymptotically optimal radius satisfies

$$\rho^*(n) = \left(\frac{n - \varsigma}{\mu \nu} \right)^{\frac{1}{\nu}}. \tag{3.22}$$

Proof. For large ρ, we have the asymptotic behaviour of the condition number

$$\kappa(n, \rho) = \frac{M(\rho)}{|a_n| \rho^n} \sim \frac{e^{\mu \rho^\nu} \rho^{\varsigma - n}}{|a_n|} = \frac{1}{|a_n|} e^{\mu \rho^\nu + (\varsigma - n) \log \rho}.$$

Direct calculation shows that the above asymptotic expression has its minimum value at $\rho = \left(\frac{n - \varsigma}{\mu \nu} \right)^{\frac{1}{\nu}}$. This completes the proof. □

Next, we consider the case where f is only analytic in a bounded region in the complex plane. Define

$$\vartheta = \sup_{1 < \rho < \rho_{\max}} \frac{\rho M'(\rho)}{M(\rho)}.$$

Furthermore, applying the third assertion of Theorem 3.3, we have

$$\vartheta = \lim_{\rho \to \rho_{\max}} \frac{\rho M'(\rho)}{M(\rho)}.$$

The following theorem is analogous to [5, Thm. 4.5], which shows the optimal radius approaches $\rho_{\max}$ for large n.

Theorem 3.7. *Let f be analytic in any ellipse $\mathcal{E}_\rho$ with $1 \le \rho < R < \infty$. Then,*

1. *If $n > \vartheta$, the condition number $\kappa^{\mathrm{Ch1}}(n,\rho)$ is strictly decreasing for $1 < \rho < \rho_{\max}$.*
2. *If $\vartheta = \infty$, then $\kappa^{\mathrm{Ch1}}(n,\rho)$ is strictly increasing in the vicinity of $\rho = \rho_{\max}$.*
3. *If $\vartheta < \infty$ and $\lim_{\rho\to\rho_{\max}} M(\rho)$ exists and is finite, then the optimal radius $\rho = \rho_{\max}$ for $n > \vartheta$.*

Proof. In analogy to [5, Thm. 4.5], differentiating the condition number with respect to ρ yields

$$\frac{d}{d\rho}\log\kappa^{\mathrm{Ch1}}(n,\rho) = \frac{M'(\rho)}{M(\rho)} - \frac{n}{\rho} \le \frac{\vartheta - n}{\rho}.$$

If $n > \vartheta$, then the condition number $\kappa^{\mathrm{Ch1}}(n,\rho)$ is a strictly decreasing function of ρ and the first assertion follows. If $\vartheta = \infty$, this implies that $\kappa^{\mathrm{Ch1}}(n,\rho)$ is strictly increasing when $\rho \to \rho_{\max}$, thus the second assertion holds. Finally, if $\vartheta < \infty$ and $\lim_{\rho\to\rho_{\max}} M(\rho)$ exists and is finite, then the third assertion follows from the first assertion. □

3.4 Examples of optimal contours

In this section we give some specific examples of optimal radii. However, first we show that the condition number accurately predicts the relative error of the Chebyshev coefficients. Fig. 1 shows the condition number, as well as the ratio of the relative error of the Chebyshev coefficients to the machine precision, for two entire functions $f(x) = e^x$ and $f(x) = \cos(2x+2)$. There is a clear agreement between both quantities. Fig. 2 shows the same experiment for two analytic functions that are not entire, $f(x) = \frac{1}{x-2}$ and $f(x) = \frac{x+1}{x^2+1}$. From this figure we observe that the condition number assumes its minimum value when ρ is close to its maximum value.

Example 3.8. Consider the exponential function $f(x) = e^x$, which is entire and transcendental. Its Chebyshev coefficients are $a_n = 2I_n(1)$ and

$$\int_0^{2\pi} \left| e^{\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})} \right| d\theta = \int_0^{2\pi} e^{\frac{1}{2}(\rho+\rho^{-1})\cos\theta} d\theta = 2\pi I_0(\tfrac{1}{2}(\rho+\rho^{-1})),$$

where $I_n(x)$ is the modified Bessel function of the first kind of order n [1, p. 376]. Thus, the condition number is

$$\kappa^{\mathrm{Ch1}}(n,\rho) = \frac{1}{I_n(1)} I_0(\tfrac{1}{2}(\rho+\rho^{-1}))\rho^{-n}. \tag{3.23}$$

Using the first term of the asymptotic expansion of the $I_n(x)$ [1, p. 377]

$$I_n(x) = \frac{e^x}{\sqrt{2\pi x}}\left(1 - \frac{4n^2-1}{8x} + \mathcal{O}(x^{-2})\right), \quad x \to \infty,$$

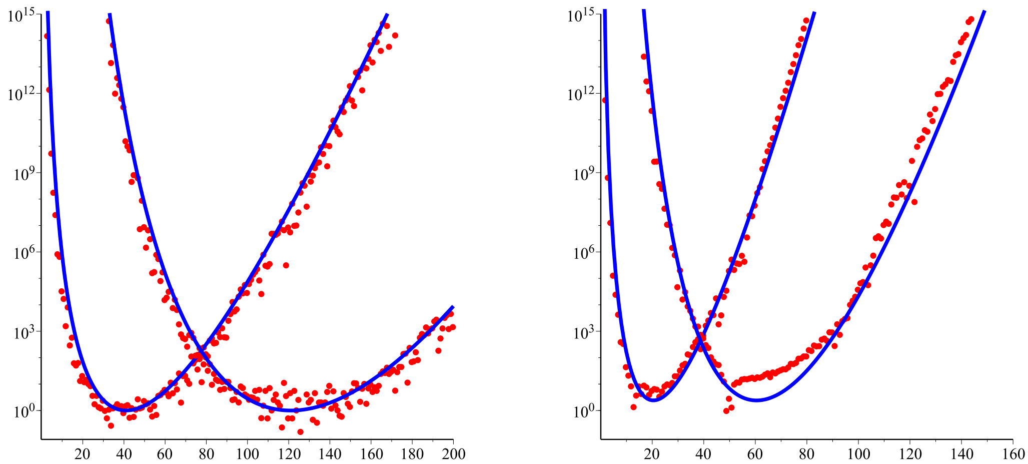

Figure 1: Ratio of the relative error of the n-th Chebtyshev coefficients to the machine precision (dots) and the condition number $\kappa(n,\rho)$ (line) for $n = 20, 60$, respectively. The test functions are $f(x) = e^x$ (left) and $f(x) = \cos(2x+2)$ (right).

we get from Theorem 3.6 that

$$\mu = \frac{1}{2}, \quad \nu = 1, \quad \varsigma = -\frac{1}{2}.$$

Therefore,

$$\rho^*(n) = 2n + 1.$$

Direct calculation of the condition number yields

$$1 \leq \kappa^{\mathrm{Ch1}}(n, 2n+1) < 1.08, \quad n \geq 0.$$

This bound for condition number shows that the Chebyshev coefficients can be accurately computed without loss of accuracy if the optimal radius is used.

Example 3.9. Consider the cosine function $f(x) = \cos(cx + d)$ with real constants c, d and $c > 0$. The exact Chebyshev coefficients are

$$a_n = 2\cos\left(d + n\frac{\pi}{2}\right) J_n(c), \quad n \geq 0,$$

where $J_n(x)$ denotes the Bessel function of the first kind. We have

$$\begin{aligned} M(\rho) &= \frac{1}{\pi}\int_0^{2\pi} \left|\cos\left(\frac{c}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) + d\right)\right| d\theta \\ &= \frac{1}{2\pi}\int_0^{2\pi} \sqrt{e^{c(\rho-\rho^{-1})\sin\theta} + e^{-c(\rho-\rho^{-1})\sin\theta} + 2\cos(c(\rho+\rho^{-1})\cos\theta + 2d)}d\theta \\ &= \frac{1}{\pi}\int_0^{\pi} \sqrt{e^{c(\rho-\rho^{-1})\sin\theta} + e^{-c(\rho-\rho^{-1})\sin\theta} + 2\cos(c(\rho+\rho^{-1})\cos\theta + 2d)}d\theta. \end{aligned}$$

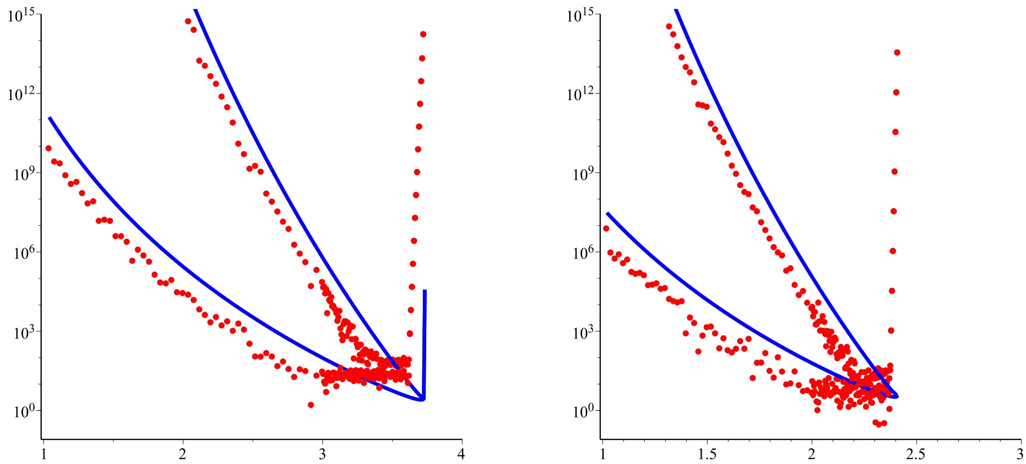

Figure 2: Ratio of the relative error of the n-th Chebyshev coefficients to the machine precision (dots) and the condition number $\kappa(n,\rho)$ (line) for $n = 20, 60$, respectively. The test functions are $f(x) = \frac{1}{x-2}$ (left) and $f(x) = \frac{x+1}{x^2+1}$ (right).

For large ρ, noting that the sum in the last equality is dominated by the first term, we have

$$\begin{aligned} M(\rho) &\sim \frac{1}{\pi}\int_0^\pi e^{\frac{c}{2}(\rho-\rho^{-1})\sin\theta} d\theta \\ &= I_0\left(\frac{c}{2}(\rho-\rho^{-1})\right) + \frac{4}{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1} I_{2k+1}\left(\frac{c}{2}(\rho-\rho^{-1})\right), \end{aligned}$$

where we have made use of the expansion [1, Eqn. 9.6.35]. Using the first term of the asymptotic expansion of $I_n(x)$, we obtain

$$M(\rho) \sim 2\frac{e^{\frac{c}{2}\rho}}{\sqrt{c\pi\rho}}, \quad \rho \to \infty.$$

Identifying with Theorem 3.6 leads to

$$\mu = \frac{c}{2}, \quad \nu = 1, \quad \varsigma = -\frac{1}{2}.$$

Thus, we can derive the optimal radius for the cosine function

$$\rho^*(n) = \frac{2n+1}{c}.$$

For example, for $c = 2$ and $d = 2$, direct calculation shows

$$1 < \kappa^{\mathrm{Ch1}}(n, \frac{2n+1}{c}) < 2.48, \quad n \geq 1.$$

Example 3.10. Consider a model function with a simple pole on the real line

$$f(x) = \frac{1}{x-a},$$

where $a > 1$. The exact Chebyshev coefficients are given by [27, Eqn. (5.14)]

$$a_n = -\frac{2}{\sqrt{a^2-1}}(a - \sqrt{a^2-1})^n, \quad n \geq 0.$$

Note that f has a pole at $z = a$, we can deduce immediately that $1 < \rho < A$ and $A = a + \sqrt{a^2-1}$. Direct calculation gives

$$\begin{aligned} M(\rho) &= \frac{1}{\pi}\int_0^{2\pi} \frac{1}{|\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1}) - a|} d\theta \\ &= \frac{2\rho}{\pi}\int_0^{2\pi} \frac{1}{|(\rho e^{i\theta})^2 - 2a(\rho e^{i\theta}) + 1|} d\theta \\ &= \frac{2\rho}{\pi}\int_0^{2\pi} \frac{1}{|(\rho e^{i\theta} - A)(\rho e^{i\theta} - A^{-1})|} d\theta. \end{aligned}$$

The latter integral can be evaluated exactly in terms of elliptic integrals. An asymptotic expression for ρ tending to A is

$$M(\rho) \sim \frac{4\rho}{\pi}\frac{3\log 2 + \log(A(A^2-1)) - \log(A^2+1) - \log(A-\rho)}{A^2-1}.$$

Optimizing the condition number for large n leads, after further asymptotic approximations, to

$$\rho^*(n) = A\left(1 - \frac{1}{n(3\,\log 2 + \log n)}\right).$$

For small values of A and n, a slightly more accurate expression is

$$\rho^*(n) = A\left(1 - \frac{1}{n(3\,\log 2 - \log(A^2+1) + \log(A^2-1) + \log n)}\right).$$

This leads for both expressions to a logarithmic growth of the condition number as a function of n, approximately $\log n/\pi$. Similar growth was observed for the computation of high derivatives of this function in [5, Example 5.2].

For example, when $a = 2$ direct calculation shows

$$1 < \kappa^{\mathrm{Ch1}}(n, \rho^*(n)) < 4.72, \quad 0 \leq n \leq 10000,$$

if we choose the optimal radius

$$\rho^*(n) = \begin{cases} A\left(1 - \frac{1}{n(3\log 2 + \log n)}\right), & \text{if } n \geq 1, \\ A\left(1 - \frac{1}{3\log 2}\right), & \text{if } n = 0. \end{cases} \tag{3.24}$$

The case where f has a complex pole can be analyzed similarly, but is slightly more involved. Expression (3.24) for the optimal radius continues to hold for a pole at the point z_0, with

$$A = |z_0 \pm \sqrt{z_0^2 - 1}|$$

and where the sign is chosen such that $A > 1$. We omit the details of the derivation.

Remark 3.11. In order to achieve the relative error tolerance ϵ by using the optimal radius, numerical experiments suggest that we need about

$$m_\epsilon \approx n(3\log 2 + \log n)\log \epsilon^{-1} \tag{3.25}$$

nodes for large n. For example, we consider the computation of a_{100} of the function $f(x) = \frac{1}{x-4}$. To achieve relative error $\epsilon = 10^{-13}$, we need $m_\epsilon \approx 20009$ nodes. Numerical results show that the relative error is 2.0×10^{-14} when $m = 20010$.

Example 3.12. Consider the function

$$f(x) = (c-x)^\phi g(x),$$

where $\phi > 0$ is not an integer and $c > 1$ and $g(x)$ is an analytic function at $x = c$. In this example, $f(x)$ has a branch point at $x = c$. Direct calculations show that the maximum value of ρ is $\rho_{\max} = c + \sqrt{c^2-1}$ and

$$\begin{aligned} M(\rho) &= \frac{1}{\pi}\int_0^{2\pi} \left| f\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)\right| d\theta \\ &= \frac{1}{\pi}\int_0^{2\pi} \left| \left(c - \frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)^\phi g\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)\right| d\theta \\ &= \frac{1}{\pi}\int_0^{2\pi} \left[\frac{1}{4}(\rho^2 + \rho^{-2}) - c(\rho + \rho^{-1})\cos\theta + \frac{1}{2}\cos(2\theta) + c^2\right]^{\frac{\phi}{2}} \\ &\qquad\qquad \left| g\left(\frac{1}{2}(\rho e^{i\theta} + (\rho e^{i\theta})^{-1})\right)\right| d\theta. \end{aligned} \tag{3.26}$$

It is easy to see that the integral in the last equation is bounded when $\rho = \rho_{\max}$. Applying Theorem 3.3 we have

$$\lim_{\rho\to\rho_{\max}} \kappa^{\mathrm{Ch1}}(n,\rho) = \frac{\lim_{\rho\to\rho_{\max}} M(\rho)}{|a_n|\rho_{\max}^n},$$

and the limit is finite. Thus, from Theorem 3.7, we deduce that the optimal radius is $\rho^*(n) = \rho_{\max}$ for large n. Moreover, from [15, Eqn. (37)] we know that the Chebyshev coefficients of $f(x)$ have the following estimate

$$a_n \simeq -\frac{2\sin(\phi\pi)(c^2-1)^{\frac{\phi}{2}} g(c)\Gamma(\phi+1)}{\pi n^{\phi+1}\rho_{\max}^n}.$$

Thus, we can estimate the growth of the optimal condition number

$$\kappa^{\mathrm{Ch1}}(n,\rho^*(n)) = \frac{M(\rho)}{|a_n|\rho_{\max}^n} \sim \mathcal{O}(n^{\phi+1}), \quad n\to\infty.$$

which shows the optimal condition number grows algebraically as $n \to \infty$.

3.5 Identifying Chebyshev coefficients with Taylor coefficients

An alternative way to reuse the results of [5] is to put the integral representation of the Chebyshev coefficients (2.5) into the form of a Cauchy integral like (1.1). We will show that this can be achieved by a conformal map. The main advantage is that theoretical results can be reused. However, this identification between integrals does not seem to lead to a new or improved numerical scheme.

Let us first show that the Chebyshev coefficients of an analytic function can be viewed as the Taylor coefficients of another analytic function. An explicit form of this function can be established in terms of a contour integral of $f(z)$.

Theorem 3.13. *Suppose that a_k are the Chebyshev coefficients of the first kind of the function $f(z)$ which is analytic inside and on the ellipse $\mathcal{E}_\rho$. Then they are the Taylor coefficients of the following function*

$$H(x) = \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} du, \tag{3.27}$$

and $H(x)$ is analytic inside the circle $\mathcal{C}_\rho$.

Proof. Suppose a_k are the Chebyshev coefficients of f and meanwhile the Taylor coefficients of another function $H(x)$, e.g.

$$f(x) = {\sum_{k=0}^{\infty}}' a_k T_k(x), \quad H(x) = \sum_{k=0}^{\infty} a_k x^k.$$

In view of the contour integral expression of a_k, we have

$$\begin{aligned} H(x) &= \sum_{k=0}^{\infty} a_k x^k \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} f(z) \sum_{k=0}^{\infty} x^k u^{-k-1} du \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{f(z)}{u-x} du \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} du. \end{aligned} \tag{3.28}$$

This completes the proof. □

Corollary 3.14. *Suppose that b_k are the Chebyshev coefficients of the second kind of the function $f(z)$ which is analytic inside and on the ellipse $\mathcal{E}_\rho$, then they are the Taylor coefficients of the following function*

$$H(x) = \frac{1}{2\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} (1-u^{-2}) du, \tag{3.29}$$

and $H(x)$ is analytic inside the circle $\mathcal{C}_\rho$.

In the following we present some concrete examples, where $H(x)$ can be deduced in (almost) closed form.

Example 3.15. Consider the exponential function $f(x) = e^x$. We have

$$H(x) = \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{e^{\frac{1}{2}(u+u^{-1})}}{u - x} du. \tag{3.30}$$

Direct calculations show that

$$\begin{aligned} a_k &= \frac{H^{(k)}(0)}{k!} \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} e^{\frac{1}{2}(u+u^{-1})} \frac{1}{(u-x)^{k+1}} du \\ &= \sum_{m=0}^{\infty} \frac{2}{2^{k+2m}\Gamma(k+m+1)\Gamma(m+1)} \\ &= 2I_k(1). \end{aligned} \tag{3.31}$$

Thus, we have

$$H(x) = 2\sum_{k=0}^{\infty} I_k(1) x^k,$$

which is an entire function.

Example 3.16. Consider the function

$$f(x) = \frac{1}{x-a}, \quad a > 1.$$

Using the residue theorem, we obtain

$$\begin{aligned} H(x) &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} du \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{2u}{u^2 - 2au + 1} \frac{1}{u-x} du \\ &= \frac{2(a+\sqrt{a^2-1})}{(x-(a+\sqrt{a^2-1}))\sqrt{a^2-1}}, \end{aligned} \tag{3.32}$$

and $H(x)$ is analytic inside the circle $|z| < a + \sqrt{a^2-1}$.

Example 3.17. Consider the following function

$$f(x) = \frac{1}{x^2+a^2}, \quad a > 0,$$

which has a pair of simple poles at $x = \pm ai$. Again, using the residue theorem yields

$$\begin{aligned} H(x) &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\frac{1}{2}(u+u^{-1}))}{u-x} du \\ &= \frac{1}{\pi i} \oint_{\mathcal{C}_\rho} \frac{4u^2}{(u^4+(4a^2+2)u^2+1)(u-x)} du \\ &= \frac{2(a+\sqrt{a^2+1})^2}{(x^2+(a+\sqrt{a^2+1})^2)a\sqrt{a^2+1}}, \end{aligned} \tag{3.33}$$

and $H(x)$ is analytic inside the circle $|z| < a + \sqrt{a^2+1}$.

4 Jacobi and Chebyshev coefficients

In this section, we describe a way to compute the coefficients of Jacobi expansions from the coefficients of a Chebyshev expansion. Implementation details are discussed in the following sections.

4.1 Jacobi polynomials

We recall a few basic facts about Jacobi polynomials in order to establish notation. The Jacobi weight function $\omega^{(\alpha,\beta)}(x)$ is defined by

$$\omega^{(\alpha,\beta)}(x) = (1-x)^\alpha (1+x)^\beta, \quad \alpha, \beta > -1.$$

The Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ of degree n is orthogonal to all polynomials of smaller degree with respect to $\omega^{(\alpha,\beta)}(x)$ on $[-1,1]$,

$$\int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x) dx = h_n^{(\alpha,\beta)} \delta_{mn}, \tag{4.1}$$

where δ_{mn} is the Kronecker delta and

$$h_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)n!}. \tag{4.2}$$

We define the inner product and the associated norm

$$\langle f, g \rangle_{\omega^{(\alpha,\beta)}} = \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) f(x) g(x) dx, \qquad \|f\| = \langle f, f \rangle_{\omega^{(\alpha,\beta)}}^{\frac{1}{2}}. \tag{4.3}$$

Let $L^2_{\omega^{(\alpha,\beta)}}$ denote the space of functions $f : [-1,1] \to \mathbb{R}$ such that $\|f\| < \infty$. Assume that $f(x) \in L^2_{\omega^{(\alpha,\beta)}}$, the Jacobi spectral expansion of f is

$$f(x) = \sum_{k=0}^{\infty} a_k^{(\alpha,\beta)} P_k^{(\alpha,\beta)}(x), \tag{4.4}$$

where $a_k^{(\alpha,\beta)}$ denotes the Jacobi spectral expansion coefficients given explicitly by

$$a_k^{(\alpha,\beta)} = \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) f(x) P_k^{(\alpha,\beta)}(x) dx, \quad k \geq 0. \tag{4.5}$$

In practice, it is of course necessary to truncate the infinite series on the right hand side of (4.4) after a suitable number of terms, e.g.

$$f_N(x) = \sum_{k=0}^{N} a_k^{(\alpha,\beta)} P_k^{(\alpha,\beta)}(x).$$

4.2 From Chebyshev expansions to Jacobi expansions

Substituting the Chebyshev expansion of the first kind into (4.5) yields

$$\begin{aligned} a_k^{(\alpha,\beta)} &= \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) f(x) P_k^{(\alpha,\beta)}(x) dx \\ &= \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) \left({\sum_{k=0}^{\infty}}' a_k T_k(x) \right) P_k^{(\alpha,\beta)}(x) dx \\ &= \sum_{m=0}^{\infty} \tau_{k+m,k}^{(\alpha,\beta)} a_{k+m} \epsilon_{k+m}. \end{aligned} \tag{4.6}$$

where $\epsilon_0 = \frac{1}{2}$, $\epsilon_n = 1$ for $n \geq 1$ and

$$\tau_{j,k}^{(\alpha,\beta)} = \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) T_j(x) dx, \quad j \geq k, \tag{4.7}$$

are the connection coefficients between Jacobi polynomials and Chebyshev polynomials of the first kind. On the other hand, substituting the Chebyshev expansion of the second kind into the Jacobi coefficients yields

$$\begin{aligned} a_k^{(\alpha,\beta)} &= \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) f(x) P_k^{(\alpha,\beta)}(x) dx \\ &= \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) \left(\sum_{k=0}^{\infty} b_k U_k(x) \right) P_k^{(\alpha,\beta)}(x) dx \\ &= \sum_{m=0}^{\infty} b_{k+m} \sigma_{k+m,k}^{(\alpha,\beta)}, \end{aligned} \tag{4.8}$$

where we have used the orthogonality of the Jacobi polynomial and

$$\sigma_{j,k}^{(\alpha,\beta)} = \frac{1}{h_k^{(\alpha,\beta)}} \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) U_j(x) dx \tag{4.9}$$

are the connection coefficients between Jacobi polynomials and Chebyshev polynomials of the second kind.

From (2.5) and (2.10) we have immediately that, for $n \geq 0$,

$$|a_n| \leq \frac{2\mathcal{M}}{\rho^n}, \quad |b_n| \leq \frac{\mathcal{M}L(\mathcal{E}_\rho)}{\pi\rho^{n+1}}, \tag{4.10}$$

where $L(\mathcal{E}_\rho)$ denotes the length of the circumference of $\mathcal{E}_\rho$. Moreover, for large values of j, as will be shown later, these connection coefficients $\tau_{j,k}^{(\alpha,\beta)}$ and $\sigma_{j,k}^{(\alpha,\beta)}$ behave like $\mathcal{O}(j^{-\mu})$ for some μ which depends on α and β. Thus, the Jacobi spectral expansion coefficients can be reasonably approximated by truncating the above series after a few terms.

Remark 4.1. The idea of using Chebyshev expansions of the first kind to compute the Legendre expansion coefficients is not new and has been proposed. e.g., by Piessens in [32] and by Xiang in [38]. The algorithms in [7, 24] for computing the Legendre and ultraspherical expansion coefficients are related to the Chebyshev expansion of the second kind.

5 Connection coefficients

In the following we shall present a hypergeometric representation and a three term recurrence formula for the connection coefficients between Jacobi and Chebyshev polynomials of the first and second kinds.

5.1 Hypergeometric representation

Lemma 5.1. *Assume that*

$$P_n^{(\gamma,\delta)}(x) = \sum_{k=0}^{n} c_{n,k}^{(\alpha,\beta)} P_k^{(\alpha,\beta)}(x).$$

Then the connection coefficients $c_{n,k}^{(\alpha,\beta)}$ *are given by*

$$\begin{aligned} c_{n,k}^{(\alpha,\beta)} &= \frac{(n+\gamma+\delta+1)_k(k+\gamma+1)_{n-k}(2k+\alpha+\beta+1)\Gamma(k+\alpha+\beta+1)}{(n-k)!\Gamma(2k+\alpha+\beta+2)} \\ &\quad \cdot {}_3\mathrm{F}_2\left[\begin{matrix} k-n, & n+k+\gamma+\delta+1, & k+\alpha+1 \\ k+\gamma+1, & 2k+\alpha+\beta+2 & \end{matrix}; 1\right]. \end{aligned} \tag{5.1}$$

The hypergeometric function ${}_3\mathrm{F}_2$ *is defined as follows*

$${}_3\mathrm{F}_2\left[\begin{matrix} a_1, & a_2, & a_3 \\ b_1, & b_2 & \end{matrix}; z\right] = \sum_{k=0}^{\infty} \frac{(a_1)_k(a_2)_k(a_3)_k}{(b_1)_k(b_2)_k} \frac{z^k}{k!}.$$

where the Pochhammer symbol $(z)_n$ *is defined as* $(z)_0 = 1$, $(z)_n = (z)_{n-1}(z+n-1)$, $n \geq 1$.

Proof. The proof is a classic result in special functions (see [3, p. 357]). □

Lemma 5.1 shows that one family of Jacobi polynomials $P_n^{(\gamma,\delta)}(x)$ can be expressed by a linear combination of another sequence of Jacobi polynomials $\{P_k^{(\alpha,\beta)}(x)\}_{k=0}^n$, with the corresponding connection coefficients expressed in terms of hypergeometric functions. Since the Chebyshev polynomials of the first and second kinds are a scalar multiple of a special case of Jacobi polynomials, we can immediately derive the connection coefficients $\tau_{j,k}^{(\alpha,\beta)}$ and $\sigma_{j,k}^{(\alpha,\beta)}$.

Theorem 5.2. *Let $\tau_{j,k}^{\alpha,\beta}$ and $\sigma_{j,k}^{\alpha,\beta}$ be defined by (4.7) and (4.9) respectively. For $j \geq k$, we have*

$$\tau_{j,k}^{(\alpha,\beta)} = \frac{j\Gamma(\frac{1}{2})\Gamma(j+k)\Gamma(k+\alpha+\beta+1)}{\Gamma(k+\frac{1}{2})\Gamma(j-k+1)\Gamma(2k+\alpha+\beta+1)} \cdot {}_3\mathrm{F}_2\left[\begin{matrix} k-j, & j+k, & k+\alpha+1 \\ k+\frac{1}{2}, & 2k+\alpha+\beta+2 & \end{matrix};1\right], \tag{5.2}$$

and $\tau_{0,0}^{(\alpha,\beta)} = 1$. Also,

$$\sigma_{j,k}^{(\alpha,\beta)} = \frac{\Gamma(\frac{3}{2})\Gamma(j+k+2)\Gamma(k+\alpha+\beta+1)}{\Gamma(k+\frac{3}{2})\Gamma(j-k+1)\Gamma(2k+\alpha+\beta+1)} \cdot {}_3\mathrm{F}_2\left[\begin{matrix} k-j, & j+k+2, & k+\alpha+1 \\ k+\frac{3}{2}, & 2k+\alpha+\beta+2 & \end{matrix};1\right]. \tag{5.3}$$

Proof. For $j \geq 0$, we have [36, p. 80]

$$T_j(x) = \frac{\Gamma(j+1)\Gamma(\frac{1}{2})}{\Gamma(j+\frac{1}{2})} P_j^{(-\frac{1}{2},-\frac{1}{2})}(x), \tag{5.4}$$

and

$$U_j(x) = \frac{\Gamma(j+2)\Gamma(\frac{3}{2})}{\Gamma(j+\frac{3}{2})} P_j^{(\frac{1}{2},\frac{1}{2})}(x). \tag{5.5}$$

Taking $\gamma = \delta = -1/2$ and $\gamma = \delta = 1/2$ respectively in Lemma 5.1 and applying the orthogonality of the Jacobi polynomials yields the desired results. □

Remark 5.3. Based on the relation $U_{j+2}(x) - U_j(x) = 2T_{j+2}(x)$, these two connection coefficients are closely related by the identity

$$\sigma_{j+2,k}^{(\alpha,\beta)} - \sigma_{j,k}^{(\alpha,\beta)} = 2\tau_{j+2,k}^{(\alpha,\beta)}. \tag{5.6}$$

For computational purposes, it is impractical to calculate the connection coefficients $\tau_{j,k}^{(\alpha,\beta)}$ and $\sigma_{j,k}^{(\alpha,\beta)}$ from their hypergeometric expressions, since hypergeometric functions are generally difficult and time consuming to compute. In the following subsection we shall establish a three-term recurrence relation for these connection coefficients. This leads to a more efficient evaluation scheme.

5.2 Recurrence formulas

We describe a three term recurrence relation for the connection coefficients. We start our proof with $\sigma_{j,k}^{(\alpha,\beta)}$ since the proof for $\tau_{j,k}^{(\alpha,\beta)}$ is similar.

5.2.1 Recurrence formula for $\sigma_{j,k}^{(\alpha,\beta)}$

Theorem 5.4. *For each $j \geq 0$, the connection coefficients $\sigma_{j,k}^{(\alpha,\beta)}$ satisfy the following three-term recurrence relation*

$$A_{j,k}^{(\alpha,\beta)}\sigma_{j+1,k}^{(\alpha,\beta)} + B_{j,k}^{(\alpha,\beta)}\sigma_{j,k}^{(\alpha,\beta)} - C_{j,k}^{(\alpha,\beta)}\sigma_{j-1,k}^{(\alpha,\beta)} = 0, \tag{5.7}$$

where

$$\begin{aligned} A_{j,k}^{(\alpha,\beta)} &= j+\alpha+\beta+2-\frac{k(k+\alpha+\beta+1)}{j+1}, \\ B_{j,k}^{(\alpha,\beta)} &= 2(\alpha-\beta), \\ C_{j,k}^{(\alpha,\beta)} &= j-\alpha-\beta-\frac{k(k+\alpha+\beta+1)}{j+1}. \end{aligned}$$

The first two initial values are given by

$$\sigma_{k-1,k}^{(\alpha,\beta)} = 0, \qquad \sigma_{k,k}^{(\alpha,\beta)} = \frac{2^{2k}\Gamma(k+1)\Gamma(k+\alpha+\beta+1)}{\Gamma(2k+\alpha+\beta+1)}, \quad k \geq 0.$$

Proof. The case $j = 0$ can be easily verified. Next we consider the case $j \geq 1$. We introduce the following auxiliary variable

$$\varsigma_{j,k}^{(\alpha,\beta)} = \frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha,\beta+1)}(x)P_k^{(\alpha,\beta)}(x)U_j(x)dx. \tag{5.8}$$

Using the properties of the Chebyshev polynomials of the second kind we immediately obtain

$$\varsigma_{j,k}^{(\alpha,\beta)} = \frac{1}{2}\sigma_{j+1,k}^{(\alpha,\beta)} + \sigma_{j,k}^{(\alpha,\beta)} + \frac{1}{2}\sigma_{j-1,k}^{(\alpha,\beta)}. \tag{5.9}$$

On the other hand, using integration by parts in (5.8) it follows that

$$\begin{aligned} \varsigma_{j,k}^{(\alpha,\beta)} &= \frac{\beta+1}{\alpha+1}\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta)}(x)P_k^{(\alpha,\beta)}(x)U_j(x)dx \\ &+ \frac{1}{\alpha+1}\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)}(x){U_j}'(x)dx \\ &+ \frac{1}{\alpha+1}\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta+1)}(x){P_k^{(\alpha,\beta)}}'(x)U_j(x)dx. \end{aligned} \tag{5.10}$$

For the first integral in (5.10), we have

$$\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta)}(x)P_k^{(\alpha,\beta)}(x)U_j(x)dx = -\frac{1}{2}\sigma_{j+1,k}^{(\alpha,\beta)} + \sigma_{j,k}^{(\alpha,\beta)} - \frac{1}{2}\sigma_{j-1,k}^{(\alpha,\beta)}. \tag{5.11}$$

For the second integral, we have, by using the relation $2(1-x^2)U_j{}'(x) = (j+2)U_{j-1}(x) - jU_{j+1}(x)$, for $j \geq 1$ ([27]), that

$$\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)}(x)U_j{}'(x)dx = -\frac{j}{2}\sigma_{j+1,k}^{(\alpha,\beta)} + \frac{j+2}{2}\sigma_{j-1,k}^{(\alpha,\beta)}. \tag{5.12}$$

For the last integral in (5.10), using integration by parts again, we get

$$\begin{aligned}
&\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)\prime}(x)U_j(x)dx \\
&= -\frac{1}{j+1}\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}[\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)\prime}(x)]'T_{j+1}(x)dx,
\end{aligned}$$

where we have used $T_{j+1}{}'(x) = (j+1)U_j(x)$ and $T_j(x)$ is the Chebyshev polynomial of the first kind of order j. Furthermore, note that Jacobi polynomials satisfy the following singular Sturm-Liouville equation [36, p. 61]

$$[\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)\prime}(x)]' + k(k+\alpha+\beta+1)\omega^{(\alpha,\beta)}(x)P_k^{(\alpha,\beta)}(x) = 0.$$

This implies that

$$\begin{aligned}
&\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha+1,\beta+1)}(x)P_k^{(\alpha,\beta)\prime}(x)U_j(x)dx \\
&= \frac{k(k+\alpha+\beta+1)}{j+1}\frac{1}{h_k^{(\alpha,\beta)}}\int_{-1}^{1}\omega^{(\alpha,\beta)}(x)P_k^{(\alpha,\beta)}(x)T_{j+1}(x)dx \\
&= \frac{k(k+\alpha+\beta+1)}{2(j+1)}(\sigma_{j+1,k}^{(\alpha,\beta)} - \sigma_{j-1,k}^{(\alpha,\beta)}). \qquad (5.13)
\end{aligned}$$

Substituting equations (5.11), (5.12) and (5.13) into (5.10) gives

$$\begin{aligned}
\varsigma_{j,k}^{(\alpha,\beta)} &= \frac{k(k+\alpha+\beta+1)-(j+1)(j+\beta+1)}{2(\alpha+1)(j+1)}\sigma_{j+1,k}^{(\alpha,\beta)} \\
&\quad + \frac{\beta+1}{\alpha+1}\sigma_{j,k}^{(\alpha,\beta)} + \frac{(j+1)(j-\beta+1)-k(k+\alpha+\beta+1)}{2(\alpha+1)(j+1)}\sigma_{j-1,k}^{(\alpha,\beta)}.
\end{aligned}$$

Combining this with equation (5.9) we derive the recurrence relation (5.7). This completes the proof. □

Corollary 5.5. *For the special case where $\alpha = \beta$, the Jacobi polynomials become the ultraspherical polynomials and thus the Jacobi coefficients become the ultraspherical coefficients. In this case, the three-term recurrence relation reduces to a two-term recurrence relation*

$$\sigma_{k+2m,k}^{(\alpha,\alpha)} = \frac{(k+2m)(k+2m-2\alpha-1)-k(k+2\alpha+1)}{(k+2m)(k+2m+2\alpha+1)-k(k+2\alpha+1)}\sigma_{k+2m-2,k}^{(\alpha,\alpha)}, \quad m \geq 1. \tag{5.14}$$

Moreover, $\sigma_{k+2m+1,k}^{(\alpha,\alpha)} = 0$ for $m \geq 0$.

This particular case of the transformation between different sets of ultraspherical polynomials was also described in [31, §3].

5.2.2 Recurrence formula for $\tau_{j,k}^{(\alpha,\beta)}$

Theorem 5.6. *For each $j \geq 0$, the connection coefficients $\tau_{j,k}^{(\alpha,\beta)}$ satisfy the following three-term recurrence relation*

$$\hat{A}_{j,k}^{(\alpha,\beta)}\tau_{j+1,k}^{(\alpha,\beta)} + \hat{B}_{j,k}^{(\alpha,\beta)}\tau_{j,k}^{(\alpha,\beta)} - \hat{C}_{j,k}^{(\alpha,\beta)}\tau_{|j-1|,k}^{(\alpha,\beta)} = 0, \tag{5.15}$$

where

$$\begin{aligned}
\hat{A}_{j,k}^{(\alpha,\beta)} &= j+\alpha+\beta+2-\frac{k(k+\alpha+\beta+1)}{j+1}, \\
\hat{B}_{j,k}^{(\alpha,\beta)} &= 2(\alpha-\beta), \\
\hat{C}_{j,k}^{(\alpha,\beta)} &= j-\alpha-\beta-2-\frac{k(k+\alpha+\beta+1)}{j-1}.
\end{aligned}$$

When $j = 1$, the last term in $\hat{C}_{j,k}^{(\alpha,\beta)}$ should be deleted. The first two initial values are given by

$$\tau_{k-1,k}^{(\alpha,\beta)} = 0, \quad k \geq 0,$$

and

$$\tau_{0,0}^{(\alpha,\beta)} = 1, \qquad \tau_{k,k}^{(\alpha,\beta)} = \frac{2^{2k-1}\Gamma(k+1)\Gamma(k+\alpha+\beta+1)}{\Gamma(2k+\alpha+\beta+1)}, \quad k \geq 1.$$

Proof. The proof is essentially similar to Theorem 5.4. □

Corollary 5.7. *For the case $\alpha = \beta$, the three-term recurrence relation reduces to a two-term recurrence relation*

$$\tau_{k+2m,k}^{(\alpha,\alpha)} = \frac{(k+2m)[(k+2m-2)(k+2m-2\alpha-3)-k(k+2\alpha+1)]}{(k+2m-2)[(k+2m)(k+2m+2\alpha+1)-k(k+2\alpha+1)]}\tau_{k+2m-2,k}^{(\alpha,\alpha)}, \tag{5.16}$$

where $k, m \geq 1$. Moreover, $\tau_{k+2m+1,k}^{(\alpha,\alpha)} = 0$ for $m \geq 0$. For the special case $\alpha = 0$, then the Jacobi polynomial becomes the Legendre polynomial and $\tau_{j,k}^{(0,0)}$ is the connection coefficient between Legendre and Chebyshev polynomials of the first kind. In this case, the two-term recurrence relation of $\tau_{j,k}^{(0,0)}$ has been given by Piessens in [32].

5.3 Asymptotics of connection coefficients

In this subsection we are interested in the asymptotics of the connection coefficients for large j. First we shall recall an asymptotic expansion for oscillatory integrals with endpoint singularities [16].

Lemma 5.8. *Suppose that*

$$f(x) = (x-a)^{\gamma}(b-x)^{\delta} g(x)$$

with $\gamma, \delta > -1$ *and* $g(x)$ *is* n *times continuously differentiable for* $x \in [a, b]$*. Furthermore, define*

$$\phi(x) = (x-a)^{\gamma} g(x), \quad \psi(x) = (b-x)^{\delta} g(x).$$

Then for large λ*,*

$$\begin{aligned}\int_a^b f(x) e^{i\lambda x} dx \sim e^{i\lambda a} \sum_{s=0}^{n-1} \frac{\psi^{(s)}(a) e^{i\frac{\pi}{2}(s+\gamma+1)} \Gamma(s+\gamma+1)}{\lambda^{s+\gamma+1} s!} \\ - e^{i\lambda b} \sum_{s=0}^{n-1} \frac{\phi^{(s)}(b) e^{i\frac{\pi}{2}(s-\delta+1)} \Gamma(s+\delta+1)}{\lambda^{s+\delta+1} s!} \\ + \mathcal{O}(\lambda^{-n-1-\min\{\gamma,\delta\}}), \quad \lambda \to \infty. \end{aligned} \tag{5.17}$$

The following lemma will be useful in proving the asymptotic of $\sigma_{j,k}^{(\alpha,\beta)}$.

Lemma 5.9. *We have*

$$\int_0^{\infty} \frac{\sin(\omega t)}{t^{\mu+1}} dt = \begin{cases} \frac{\Gamma(1-\mu)\sin(\frac{\pi}{2}\mu)}{\mu} \omega^{\mu}, & \text{if } 0 < \mu < 1, \\ \frac{\pi}{2}, & \text{if } \mu = 0. \end{cases} \tag{5.18}$$

Proof. The case $\mu = 0$ is obvious. For $0 < \mu < 1$, using integration by parts yields

$$\int_0^{\infty} \frac{\sin(\omega t)}{t^{\mu+1}} dt = \frac{\omega}{\mu} \int_0^{\infty} \frac{\cos(\omega t)}{t^{\mu}} dt.$$

In view of the formal identity [30, Lemma 12.1]

$$\int_0^{\infty} \frac{e^{i\omega t}}{t^{\mu}} dt = \frac{\Gamma(1-\mu)}{\omega^{1-\mu}} e^{\frac{\pi}{2}(1-\mu)i},$$

taking the real part of the above integral yields the result. □

Theorem 5.10. *Suppose* $\alpha, \beta > -1$*. If neither* 2α *nor* 2β *is a positive odd integer, then for large* j*, we have*

$$\sigma_{j,k}^{(\alpha,\beta)} \sim \mathcal{O}(j^{-2\min\{\alpha,\beta\}-1}). \tag{5.19}$$

Furthermore, if one of 2α and 2β is a positive odd integer, then

$$\sigma_{j,k}^{(\alpha,\beta)} = \begin{cases} \mathcal{O}(j^{-2\beta-1}), & \text{if } 2\alpha \text{ is positive odd,} \\ \mathcal{O}(j^{-2\alpha-1}), & \text{if } 2\beta \text{ is positive odd.} \end{cases} \tag{5.20}$$

If both 2α and 2β are positive odd integers and $2\alpha = 2k_1+1$, $2\beta = 2k_2+1$, for $k_1, k_2 \geq 0$, then

$$\sigma_{j,k}^{(\alpha,\beta)} = 0, \quad j \geq k + k_1 + k_2 + 1. \tag{5.21}$$

Proof. Letting $x = \cos\theta$, we have

$$\begin{aligned} h_k^{(\alpha,\beta)} \sigma_{j,k}^{(\alpha,\beta)} &= \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) U_j(x) dx \\ &= \int_0^{\pi} \theta^{2\alpha} (\pi-\theta)^{2\beta} \hat{g}(\theta) \sin(j+1)\theta d\theta, \end{aligned} \tag{5.22}$$

where

$$\hat{g}(\theta) = 2^{\alpha+\beta} (\theta^{-1} \sin\tfrac{\theta}{2})^{2\alpha} ((\pi-\theta)^{-1} \cos\tfrac{\theta}{2})^{2\beta} P_k^{(\alpha,\beta)}(\cos\theta).$$

It is clear that $\hat{g}(\theta)$ is regular at both endpoints. Define the following two auxiliary functions

$$\hat{\psi}(\theta) = (\pi-\theta)^{2\beta} \hat{g}(\theta), \quad \hat{\phi}(\theta) = \theta^{2\alpha} \hat{g}(\theta). \tag{5.23}$$

Obviously, $\hat{\psi}(\theta)$ and $\hat{\phi}(\theta)$ are regular at $\theta = 0$ and $\theta = \pi$, respectively. Furthermore, straightforward calculation confirms that

$$\hat{\psi}^{(2s+1)}(0) = 0, \quad \hat{\phi}^{(2s+1)}(\pi) = 0, \quad s = 0, 1, \ldots \tag{5.24}$$

Combining these with Lemma 5.8, we obtain for $\alpha, \beta > -\frac{1}{2}$ that

$$\begin{aligned} h_k^{(\alpha,\beta)} \sigma_{j,k}^{(\alpha,\beta)} &= \int_0^{\pi} \theta^{2\alpha} (\pi-\theta)^{2\beta} \hat{g}(\theta) \sin(j+1)\theta d\theta \\ &= \cos(\alpha\pi) \sum_{s=0}^{\infty} (-1)^s \frac{\hat{\psi}^{(2s)}(0) \Gamma(2\alpha+2s+1)}{(j+1)^{2s+2\alpha+1}(2s)!} \\ &\quad + (-1)^j \cos(\beta\pi) \sum_{s=0}^{\infty} (-1)^s \frac{\hat{\phi}^{(2s)}(\pi) \Gamma(2\beta+2s+1)}{(j+1)^{2s+2\beta+1}(2s)!}, \quad j \to \infty. \end{aligned} \tag{5.25}$$

Thus, if neither 2α nor 2β are positive odd integers, then (5.19) holds. Furthermore, if either 2α or 2β is a positive odd integer, then (5.20) holds by noting that $\cos(\frac{k}{2}\pi) = 0$ for $k = 1, 3, \ldots$. If both 2α and 2β are positive odd integers and $2\alpha = 2k_1+1$, $2\beta = 2k_2+1$, for $k_1, k_2 = 0, 1, \ldots$, then

$$\begin{aligned} h_k^{(\alpha,\beta)} \sigma_{j,k}^{(\alpha,\beta)} &= \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) U_j(x) dx \\ &= \int_{-1}^{1} \sqrt{1-x^2} P_k^{(\alpha,\beta)}(x) (1-x)^{k_1} (1+x)^{k_2} U_j(x) dx. \end{aligned} \tag{5.26}$$

Since the polynomial $(1-x)^{k_1}(1+x)^{k_2}U_j(x)$ can be written as a linear combination of $U_{j-k_1-k_2}(x)$, $U_{j-k_1-k_2+1}(x)$, …, $U_{j+k_1+k_2}(x)$, and because of the orthogonality properties of the Chebyshev polynomials of the second kind we find that

$$\sigma_{j,k}^{(\alpha,\beta)} = 0, \quad j \geq k_1 + k_2 + k + 1.$$

If either α or β is less than or equal to $-1/2$, then Lemma 5.8 can not be used for (5.22) since 2α or 2β will be less than or equal to -1. We consider the case $-1 < \alpha \leq -\frac{1}{2} < \beta$. We first split the integral into two parts

$$\begin{aligned} h_k^{(\alpha,\beta)}\sigma_{j,k}^{(\alpha,\beta)} &= \int_0^\pi \theta^{2\alpha}(\pi-\theta)^{2\beta}\hat{g}(\theta)\sin(j+1)\theta d\theta \\ &= \int_0^{\frac{\pi}{2}} \theta^{2\alpha}\hat{\psi}(\theta)\sin(j+1)\theta d\theta + \int_{\frac{\pi}{2}}^{\pi} (\pi-\theta)^{2\beta}\hat{\phi}(\theta)\sin(j+1)\theta d\theta. \end{aligned} \tag{5.27}$$

We use S_1 and S_2 denote the first and second integrals of the last equality, respectively. For S_2, the integrand is regular at the left endpoint $\theta = \frac{\pi}{2}$. Then, using Lemma 5.8 we can deduce directly that if 2β is not a positive integer,

$$S_2 = \begin{cases} \mathcal{O}(j^{-\min\{1,2\beta+1\}}), & \text{if } j \text{ is odd,} \\ \mathcal{O}(j^{-\min\{2,2\beta+1\}}), & \text{if } j \text{ is even.} \end{cases}$$

If 2β is a positive integer, then note that $\cos(\beta\pi) = 0$ and

$$S_2 = \begin{cases} \mathcal{O}(j^{-1}), & \text{if } j \text{ is odd,} \\ \mathcal{O}(j^{-2}), & \text{if } j \text{ is even.} \end{cases}$$

In the following we shall consider the asymptotic of S_1. Direct calculation yields

$$\hat{\psi}(\theta) = 2^{\beta-\alpha}P_k^{(\alpha,\beta)}(1) + \mathcal{O}(\theta^2), \quad \theta \to 0^+. \tag{5.28}$$

Moreover, it is easy to verify that

$$\int_0^{\frac{\pi}{2}} \theta^{2\alpha+2}\sin(j+1)\theta d\theta = \mathcal{O}(j^{-1}), \quad j \to \infty.$$

Substituting the expansion (5.28) into S_1 and integrating term by term, we have

$$\begin{aligned} S_1 &= 2^{\beta-\alpha}P_k^{(\alpha,\beta)}(1)\int_0^{\frac{\pi}{2}} \theta^{2\alpha}\sin(j+1)\theta d\theta + \mathcal{O}(j^{-1}) \\ &= 2^{\beta-\alpha}P_k^{(\alpha,\beta)}(1)\left(\int_0^{\infty} \theta^{2\alpha}\sin(j+1)\theta d\theta - \int_{\frac{\pi}{2}}^{\infty} \theta^{2\alpha}\sin(j+1)\theta d\theta\right) \\ &\quad + \mathcal{O}(j^{-1}). \end{aligned}$$

Using integration by parts to the second integral in the brackets, this results in

$$\begin{aligned}\int_{\frac{\pi}{2}}^{\infty} \theta^{2\alpha} \sin(j+1)\theta d\theta = &\frac{1}{j+1}\left(\frac{\pi}{2}\right)^{2\alpha} \cos\left(\frac{\pi}{2}(j+1)\right) \\ &- \frac{2\alpha}{(j+1)^2}\left(\frac{\pi}{2}\right)^{2\alpha-1} \sin\left(\frac{\pi}{2}(j+1)\right) + \mathcal{O}(j^{-3}).\end{aligned}$$

Meanwhile, from Lemma 5.9, we get, by setting $\mu = -2\alpha - 1$, that

$$\int_0^{\infty} \theta^{2\alpha} \sin(j+1)\theta d\theta = \begin{cases} \frac{\Gamma(2\alpha+2)\cos(\alpha\pi)}{2\alpha+1}(j+1)^{-2\alpha-1}, & \text{if } -1 < \alpha < -\frac{1}{2}, \\ \frac{\pi}{2}, & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Combining these we have

$$S_1 = \begin{cases} 2^{\beta-\alpha} P_k^{(\alpha,\beta)}(1) \frac{\Gamma(2\alpha+2)\cos(\alpha\pi)}{2\alpha+1}(j+1)^{-2\alpha-1} + \mathcal{O}(j^{-1}), & \text{if } -1 < \alpha < -\frac{1}{2}, \\ 2^{\beta-\alpha-1}\pi P_k^{(\alpha,\beta)}(1) + \mathcal{O}(j^{-1}), & \text{if } \alpha = -\frac{1}{2}. \end{cases} \tag{5.29}$$

It follows that

$$\begin{aligned} h_k^{(\alpha,\beta)} \sigma_{j,k}^{(\alpha,\beta)} &= S_1 + S_2 \\ &= \mathcal{O}(j^{-2\alpha-1}). \end{aligned}$$

Similarly, the case $-1 < \beta \le -\frac{1}{2} < \alpha$ can be proved. We give the result directly

$$\sigma_{j,k}^{(\alpha,\beta)} = \mathcal{O}(j^{-2\beta-1}), \quad j \to \infty.$$

Finally, if $-1 < \alpha, \beta \le -\frac{1}{2}$, we can prove in a similar way that $S_1 = \mathcal{O}(j^{-2\alpha-1})$ and $S_2 = \mathcal{O}(j^{-2\beta-1})$. Thus

$$\begin{aligned} h_k^{(\alpha,\beta)} \sigma_{j,k}^{(\alpha,\beta)} &= S_1 + S_2 \\ &= \mathcal{O}(j^{-2\min\{\alpha,\beta\}-1}). \end{aligned}$$

This completes the proof. □

Figure 3 illustrates the absolute values of the product of $j^{2\min\{\alpha,\beta\}+1}$ and $\sigma_{j,k}^{(\alpha,\beta)}$ for several different values of α and β. This figure clearly demonstrates the asymptotic order of $\sigma_{j,k}^{(\alpha,\beta)}$ for large values of j and confirms our theoretical analysis.

Remark 5.11. For the special case $\alpha = \beta = -\frac{1}{2}$, direct calculation yields

$$\sigma_{j,k}^{(\alpha,\beta)} = \begin{cases} \frac{\pi\Gamma(2k+1)}{2^{2k-1}\Gamma(k+\frac{1}{2})^2}, & \text{if } j = k + 2m \text{ and } m = 0, 1, \ldots, \\ 0, & \text{otherwise}. \end{cases} \tag{5.30}$$

Thus, for fixed k, the connection coefficients $\sigma_{j,k}^{(\alpha,\beta)}$ are bounded as j increases.

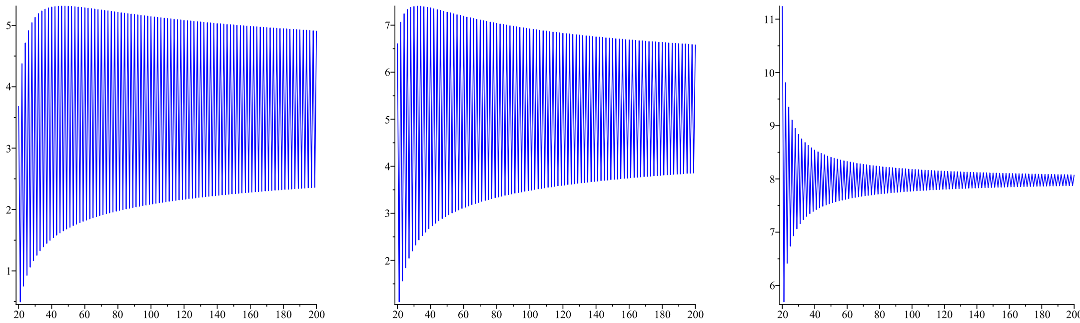

Figure 3: Absolute values of $j^{2\min\{\alpha,\beta\}+1}\sigma_{j,k}^{(\alpha,\beta)}$ for $\alpha=-\frac{2}{3},\beta=-\frac{4}{5}$ (left), $\alpha=-\frac{2}{3},\beta=-\frac{1}{2}$ (middle) and $\alpha=-\frac{1}{2},\beta=0$ (right). Here we choose $k=20$ and $j=20\dots200$.

Remark 5.12. The connection coefficients $\sigma_{j,k}^{(\alpha,\beta)}$ increase as j grows at most linearly with respect to j. Actually, for $\alpha,\beta>-1$, by using the Schwarz inequality, we get

$$\begin{aligned}|\sigma_{j,k}^{(\alpha,\beta)}| &\le \frac{1}{h_k^{(\alpha,\beta)}}\left(\int_{-1}^{1}\omega^{(\alpha,\beta)}(x)P_k^{(\alpha,\beta)}(x)^2dx\right)^{\frac{1}{2}}\left(\int_{-1}^{1}\omega^{(\alpha,\beta)}(x)U_j(x)^2dx\right)^{\frac{1}{2}}\\ &\le (j+1)\sqrt{\frac{h_0^{(\alpha,\beta)}}{h_k^{(\alpha,\beta)}}},\end{aligned}\tag{5.31}$$

where we have used the fact that $|U_j(x)|\le j+1$ for $j\ge0$.

Remark 5.13. In analogy to Theorem 5.10, the asymptotic of $\tau_{j,k}$ for large j can be established; see Appendix A.

6 Fast algorithms to maximize the efficiency

From (4.10) we know that the two kinds of Chebyshev coefficients a_n and b_n decay exponentially. Meanwhile, the corresponding connection coefficients $\tau_{j,k}^{(\alpha,\beta)}$, $\sigma_{j,k}^{(\alpha,\beta)}$ behave like $\mathcal{O}(j^{-\mu})$ for some $\mu>-1$ which depends on α and β. This means that the Jacobi expansion coefficients can be approximated accurately by truncating the first few terms of the expansion (4.6) or (4.8). Meanwhile, by choosing the same ρ in (3.1) and (3.4), the Chebyshev coefficients a_n and b_n can be computed efficiently by a single FFT.

6.1 Chebyshev expansion of the first kind

We can truncate the infinite series on the right hand side of (4.6). This leads to an approximation approach for the Jacobi coefficients

$$\begin{aligned}\breve{a}_k^{(\alpha,\beta)} &= \sum_{m=0}^{M} \tau_{k+m,k}^{(\alpha,\beta)} a_{k+m} \epsilon_{k+m} \\ &\approx \sum_{m=0}^{M} \tau_{k+m,k}^{(\alpha,\beta)} a_{k+m}(\tilde{N},\rho) \epsilon_{k+m},\end{aligned} \tag{6.1}$$

where $\tilde{N} = N + M + 1$ and $a_{k+m}(\tilde{N},\rho)$ is defined as in (3.1).

We outline our implementation steps as follows:

Algorithm 1 Compute the Jacobi spectral coefficients $\{a_k^{(\alpha,\beta)}\}_{k=0}^{N}$

```
Input M, ρ and N
for k = 0 : N do
    for m = 0 : M do
        Compute τ_{k+m,k}^{(α,β)} by (5.15)
    end for
end for
for m = 0 : Ñ do
    Evaluate a_{k+m}(Ñ, ρ) by a single FFT
end for
Calculate {a_k^{(α,β)}}_{k=0}^N by (6.1)
```

In algorithm 1, the calculation of the connection coefficients $\tau_{k+m,k}^{(\alpha,\beta)}$ can be performed in $\mathcal{O}(MN)$ operations, and the computed Chebyshev coefficients $b_m(\tilde{N},\rho)$ can be computed in $\mathcal{O}(\tilde{N}\log\tilde{N})$ operations by a single FFT. Therefore, the total computational cost of our algorithm is $\mathcal{O}(MN) + \mathcal{O}(\tilde{N}\log\tilde{N})$ operations. Most importantly, we shall prove in the following subsection that the constant M can be chosen independently of N and this implies the proposed algorithm is a truly $\mathcal{O}(N\log N)$ algorithm, as long as a fixed accuracy ϵ is desired.

6.2 Choice of M

In the following we shall prove that M can be chosen independent of N.

Lemma 6.1. *For $\alpha,\beta > -1$, there exists a constant C such that*

$$h_0^{(\alpha,\beta)} \le Cnh_n^{(\alpha,\beta)}, \quad n \ge 1.$$

Proof. From (4.2), we have

$$\frac{h_0^{(\alpha,\beta)}}{h_n^{(\alpha,\beta)}} = \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} \times \frac{\Gamma(n+\alpha+\beta+1)\Gamma(n+1)(2n+\alpha+\beta+1)}{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}. \tag{6.2}$$

Using the Stirling's approximation

$$\Gamma(x+1) \sim \sqrt{2\pi} x^{x+\frac{1}{2}} e^{-x}, \quad x \to \infty,$$

it follows that

$$\lim_{n\to\infty} \frac{\Gamma(n+\alpha+\beta+1)\Gamma(n+1)}{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)} = 1.$$

Thus, we obtain

$$\lim_{n\to\infty} \frac{h_0^{(\alpha,\beta)}}{n h_n^{(\alpha,\beta)}} = \frac{2\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}. \tag{6.3}$$

If a sequence converges, it must be bounded. We can deduce that the quotient on the left side can be bounded by a constant C for any $n \geq 1$. This completes the proof. $\square$

Theorem 6.2. *Given a tolerance ϵ, there exists a constant M independent of N such that*

$$|a_k^{(\alpha,\beta)} - \check{a}_k^{(\alpha,\beta)}| < \epsilon, \quad k \geq 0.$$

Proof. Using the Cauchy-Schwarz inequality, we have

$$\begin{aligned}
|\tau_{j,k}^{(\alpha,\beta)}| &\leq \frac{1}{h_k^{(\alpha,\beta)}} \left(\int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x)^2 dx \right)^{\frac{1}{2}} \left(\int_{-1}^{1} \omega^{(\alpha,\beta)}(x) T_j(x)^2 dx \right)^{\frac{1}{2}} \\
&\leq \sqrt{\frac{h_0^{(\alpha,\beta)}}{h_k^{(\alpha,\beta)}}},
\end{aligned}$$

which together with (4.10) yields

$$\begin{aligned}
|a_k^{(\alpha,\beta)} - \check{a}_k^{(\alpha,\beta)}| &\leq \sum_{k=M+1}^{\infty} |a_{k+m}||\tau_{k+m,k}^{(\alpha,\beta)}| \\
&\leq \sum_{k=M+1}^{\infty} \frac{2\mathcal{M}}{\rho^{k+m}} \sqrt{\frac{h_0^{(\alpha,\beta)}}{h_k^{(\alpha,\beta)}}} \\
&= 2\mathcal{M} \sqrt{\frac{h_0^{(\alpha,\beta)}}{h_k^{(\alpha,\beta)}}} \frac{1}{\rho^{k+M}(\rho-1)}.
\end{aligned} \tag{6.4}$$

For $k = 0$, we can easily obtain

$$|a_0^{(\alpha,\beta)} - \check{a}_0^{(\alpha,\beta)}| \leq \frac{2\mathcal{M}}{\rho^M(\rho-1)}.$$

For $k \geq 1$, we have by using Lemma 6.1 that

$$|a_k^{(\alpha,\beta)} - \check{a}_k^{(\alpha,\beta)}| \leq \frac{2\mathcal{M}\sqrt{Ck}}{\rho^{k+M}(\rho-1)}.$$

Define the function $h(x) = \frac{x^\delta}{\rho^x}$ with $\delta > 0$ and $x \geq 1$. Direct calculation shows that this function reaches its maximum value at the point $\max\{1, \frac{\delta}{\log \rho}\}$. Therefore, for $k \geq 1$,

$$|a_k^{(\alpha,\beta)} - \breve{a}_k^{(\alpha,\beta)}| \leq \frac{2\mathcal{M}\sqrt{Cd_1}}{\rho^{d_1+M}(\rho-1)}.$$

where $d_1 = \max\left\{1, \frac{1}{2\log\rho}\right\}$. Let $\bar{C} = \max\{1, \sqrt{C}\frac{\sqrt{d_1}}{\rho^{d_1}}\}$, it turns out that a uniform upper bound can be derived for $k \geq 0$

$$|a_k^{(\alpha,\beta)} - \breve{a}_k^{(\alpha,\beta)}| \leq \frac{2\bar{C}\mathcal{M}}{\rho^M(\rho-1)}. \tag{6.5}$$

It follows that, for a given tolerance $\epsilon > 0$, it is sufficient to choose

$$M > \frac{\log(2\bar{C}\mathcal{M}) - \log((\rho-1)\epsilon)}{\log\rho} \tag{6.6}$$

which results in

$$|a_k^{(\alpha,\beta)} - \breve{a}_k^{(\alpha,\beta)}| \leq \epsilon, \quad k \geq 0.$$

This completes the proof. □

Remark 6.3. A lower bound for M is derived explicitly in (6.6). However, as also remarked by Iserles in [24], the lower bound for M usually overestimates significantly the smallest value of M for a given tolerance ϵ.

6.3 Chebyshev expansion of the second kind

Similarly, truncating the first few terms of (4.8) yields the approximation

$$\begin{aligned}\tilde{a}_k^{(\alpha,\beta)} &= \sum_{m=0}^{M} b_{k+m}\sigma_{k+m,k}^{(\alpha,\beta)} \\ &\approx \sum_{m=0}^{M} b_{k+m}(\tilde{N},\rho)\sigma_{k+m,k}^{(\alpha,\beta)},\end{aligned} \tag{6.7}$$

where $b_{k+m}(\tilde{N},\rho)$ is defined as in (3.4). By choosing the same value of ρ for each coefficient, the set $\{b_k\}_{k=0}^{\tilde{N}-1}$ can be computed with a single FFT and this precess can be performed in only $\mathcal{O}(\tilde{N}\log\tilde{N})$ operations.

We outline the main steps in Algorithm 2. Similarly as before, we can prove that the algorithm is an $\mathcal{O}(N\log N)$ algorithm. For more details, see Appendix B.

Algorithm 2 Compute the Jacobi spectral coefficients $\{a_k^{(\alpha,\beta)}\}_{k=0}^N$

```
Input M, ρ and N
for k = 0 : N do
    for m = 0 : M do
        Compute σ_{k+m,k}^{(α,β)} by (5.7)
    end for
end for
for m = 0 : Ñ do
    Evaluate b_m(Ñ, ρ) by a single FFT
end for
Calculate {a_k^{(α,β)}}_{k=0}^N by (6.7)
```

6.4 The ultraspherical case

When $\alpha = \beta$, the Jacobi polynomials are known as ultraspherical polynomials. With a different normalization, such polynomials are also called Gegenbauer polynomials. This is an interesting special case to consider.

Let us first consider using Chebyshev expansion of the first kind. From the parity of ultraspherical polynomials, we have immediately that

$$\tau_{k+2m+1,k}^{(\alpha,\alpha)} = 0, \quad m \geq 0.$$

and thus

$$a_k^{(\alpha,\alpha)} = \sum_{m=0}^{\infty} \tau_{k+2m,k}^{(\alpha,\alpha)} a_{k+2m} \epsilon_{k+2m}.$$

This leads to

$$\breve{a}_k^{(\alpha,\alpha)} = \sum_{m=0}^{M} \tau_{k+2m,k}^{(\alpha,\alpha)} a_{k+2m} \epsilon_{k+2m}.$$

In this case, the connection coefficients $\tau_{k+2m,k}^{(\alpha,\alpha)}$ can be computed by using the two-term recurrence relation (5.16).

In analogy to the substitution of Chebyshev polynomial of the first kind into the ultraspherical coefficients, we can substitute the Chebyshev expansion of the second kind directly into the ultraspherical coefficients and obtain a similar algorithm. After some manipulations, this approach turns out to be equivalent to the fast algorithms proposed by Cantero and Iserles [7].

7 Numerical examples I: efficiency

In this section we present some numerical experiments to illustrate the efficiency of the proposed algorithms. In order to illustrate the accuracy and errors associated with algorithms 1 and 2, they were implemented and run using MAPLE with 16-digit arithmetic.

Example 7.1. We first consider the computation of the Jacobi expansion coefficients for the three functions $f(x) = e^x$, $f(x) = \cos(2x+2)$ and $f(x) = \frac{1}{x-2}$. In Figure 4 we illustrate the error of the first 50 Jacobi coefficients with $\alpha = 1$, $\beta = 2$ and $\rho = 2$. In Figure 5 we illustrate the error with $\alpha = -\frac{1}{2}$, $\beta = 0$ and $\rho = 1$. It is clear from these two figures that more accurate approximations are obtained as M increases.

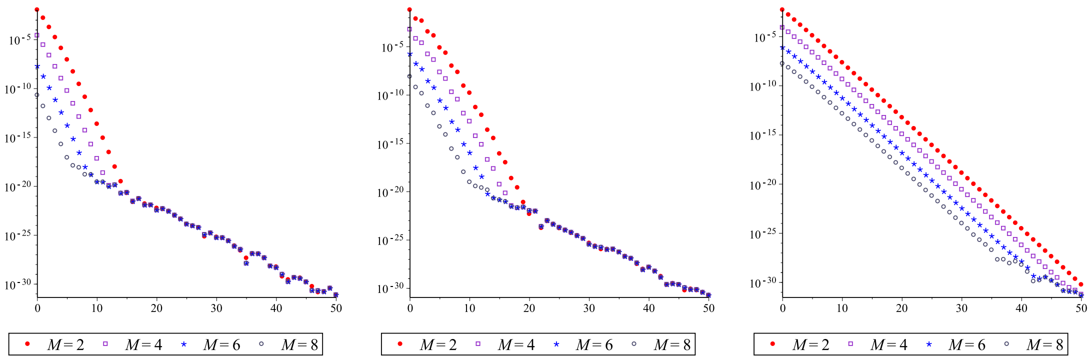

Figure 4: Absolute errors of Algorithm 1 to $f(x) = e^x$ (left), $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-2}$ (right). Here k ranges from 0 to 50.

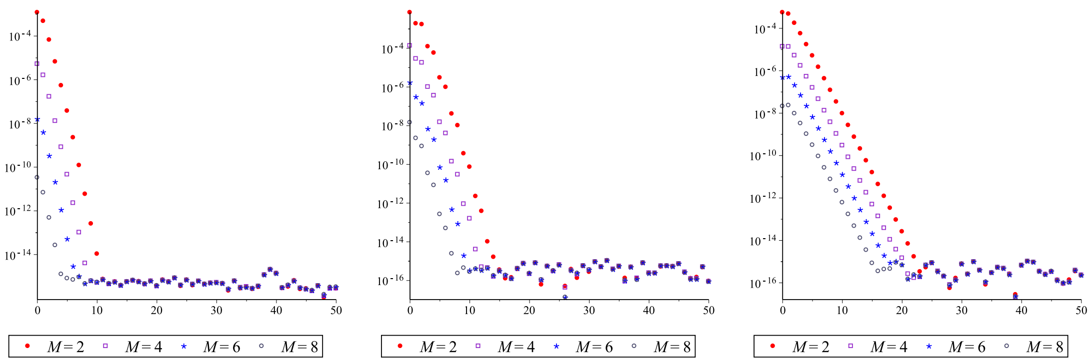

Figure 5: Absolute errors of Algorithm 1 to $f(x) = e^x$ (left), $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-2}$ (right).

Example 7.2. We compute the Jacobi coefficients of the above three functions with Algorithm 2. Numerical results are illustrated in Figures 6 and 7. Comparing Figures 4 and 6, we observe that both algorithms are of approximately equal accuracy for $\rho = 2$. Furthermore, comparing Figures 5 and 7, we can see clearly that Algorithm 2 is of equal accuracy for entire functions. For functions with a pole, however, it can be seen that Algorithm 1 is more accurate than Algorithm 2 when we choose $\rho = 1$.

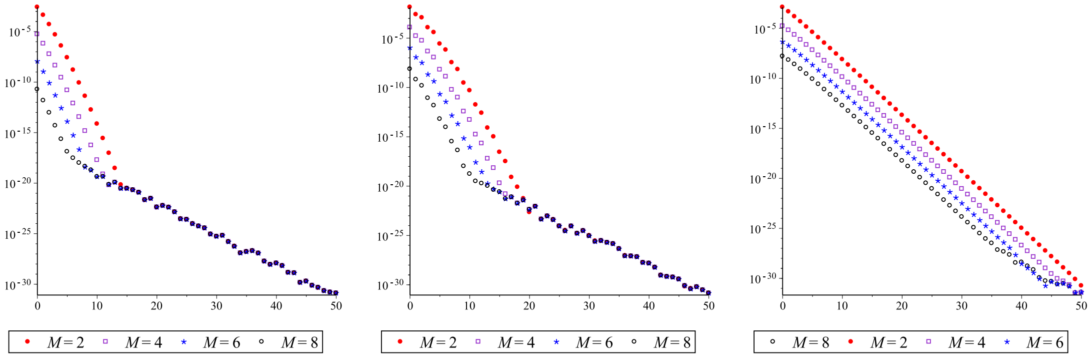

Figure 6: Absolute errors of algorithm 2 to $f(x) = e^x$ (left), $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-2}$ (right). Here $\alpha = 1$, $\beta = 2$ and k ranges from 0 to 50.

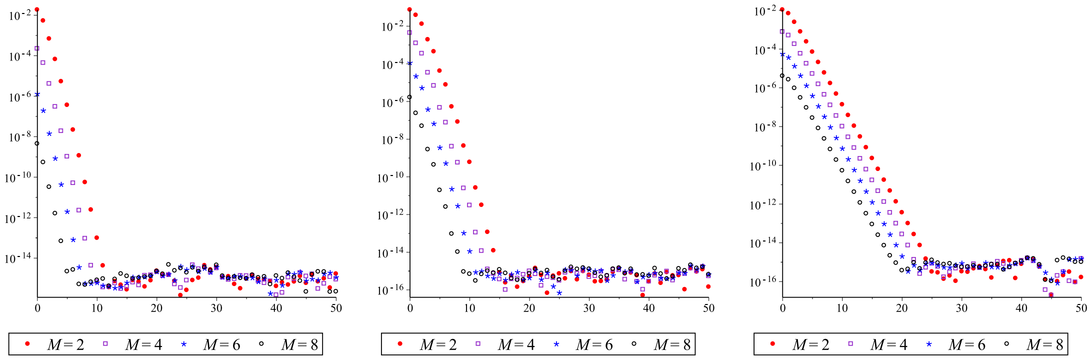

Figure 7: Absolute errors of algorithm 2 to $f(x) = e^x$ (left), $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-2}$ (right). Here $\alpha = -\frac{1}{2}$, $\beta = 0$ and k ranges from 0 to 50.

8 Maximizing the accuracy of Jacobi coefficients

In this section, we consider the computation of Jacobi coefficients with maximum accuracy. As analyzed in §3.2, there exists an optimal radius for each Chebyshev coefficient such that its relative error is small. Therefore, if we first compute each Chebyshev coefficient by using the optimal radius and then compute the Jacobi coefficients, this strategy will improve the accuracy of the Jacobi coefficients.

Theorem 8.1. *Assume that f is analytic and that the condition number of its Chebyshev coefficients* (3.13) *is bounded. Then for each ϵ perturbation of f, there exists a value of M such that the relative errors of the first N computed Jacobi coefficients are proportional to ϵ.*

Proof. Suppose $\hat{f}$ denotes the perturbation of f as in §3.2. We write the Jacobi coefficients in terms of the Chebyshev coefficients a_k as

$$a_k^{(\alpha,\beta)} = \sum_{m=0}^{\infty} a_{k+m} \tau_{k+m,k}^{(\alpha,\beta)}.$$

Then the computed Jacobi coefficients are*

$$\hat{a}_k^{(\alpha,\beta)} = \sum_{m=0}^{M} \hat{a}_{k+m} \tau_{k+m,k}^{(\alpha,\beta)}, \quad 0 \le k \le N.$$

This leads to

$$\begin{aligned}
\frac{|a_k^{(\alpha,\beta)} - \hat{a}_k^{(\alpha,\beta)}|}{|a_k^{(\alpha,\beta)}|} &\le \sum_{m=0}^{M} \left| \frac{a_{k+m} - \hat{a}_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| + \sum_{m=M+1}^{\infty} \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| \\
&\le \sum_{m=0}^{M} \left| \frac{a_{k+m} - \hat{a}_{k+m}}{a_{k+m}} \right| \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| + \sum_{m=M+1}^{\infty} \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| \\
&\le \epsilon \sum_{m=0}^{M} \kappa^{\mathrm{Ch1}}(k+m, \rho(k+m)) \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| + \sum_{m=M+1}^{\infty} \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}|.
\end{aligned}$$

If the condition number of the Chebyshev coefficients is bounded,

$$\kappa^{\mathrm{Ch1}}(n, \rho(n)) \le \kappa, \quad 0 \le n \le M+N,$$

this results in

$$\frac{|a_k^{(\alpha,\beta)} - \check{a}_k^{(\alpha,\beta)}|}{|a_k^{(\alpha,\beta)}|} \le \kappa\epsilon \sum_{m=0}^{M} \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}| + \sum_{m=M+1}^{\infty} \left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| |\tau_{k+m,k}^{(\alpha,\beta)}|.$$

Note that

$$\left| \frac{a_{k+m}}{a_k^{(\alpha,\beta)}} \right| \sim \mathcal{O}\left(\rho^{-m}\right),$$

which implies that the last sum on the right hand side behaves like $\mathcal{O}(\rho^{-M})$. Meanwhile, the first term on the right hand side behaves like $\mathcal{O}(\epsilon)$. Finally, recall that the connection coefficients τ are bounded asymptotically, as shown in Theorem A.1. Thus, we can deduce that the relative error of the Jacobi coefficients can be guaranteed to be small if we choose a sufficiently large M. This completes the proof. □

*Here we always assume that the perturbed Chebyshev coefficients and the connection coefficients are computed exactly.

9 Numerical examples II: accuracy

In the final section, we illustrate with several experiments the high accuracy in the computation of Chebyshev and Jacobi coefficients when choosing the optimal radius.

First, we illustrate the limited relative accuracy when choosing a fixed radius. Fig. 8 shows the relative error of the Jacobi coefficients $a_k^{(\alpha,\beta)}$ with $\alpha = 1$, $\beta = 2$ and $\rho = 1$. It is seen that the relative error is small only for the first several Jacobi coefficients.

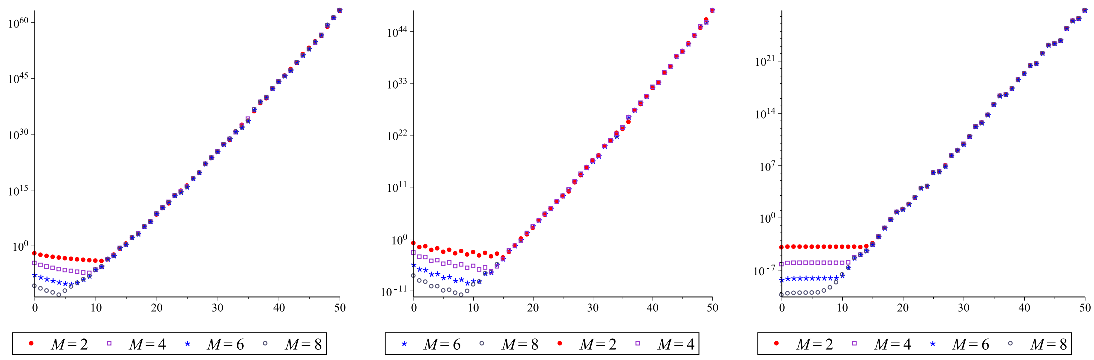

Figure 8: Relative errors of the Jacobi coefficients of $f(x) = e^x$ (left) and $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-4}$ (right) for several values of M. Here $\rho = 1$ and $m = 256$.

Example 9.1. We consider test functions $f(x) = e^x$, $f(x) = \cos(2x+2)$ and $f(x) = \frac{1}{x-4}$. We test the relative errors of the first 100 Jacobi coefficients with $\alpha = 1$ and $\beta = 2$ for several values of M. These Chebyshev coefficients are computed by the trapezoidal rule (3.1) with the optimal radius. The number of points in the trapezoidal rule is chosen to be $m = 10^2$ for the first two functions. For the last test function, each Chebyshev coefficients a_n is evaluated by the trapezoidal rule (3.1) with the number of the nodes

$$m = \max\{n(3\log 2 + \log n)\log \epsilon^{-1}, 50\}, \quad 0 \le n \le 100, \tag{9.1}$$

and $\epsilon = 10^{-13}$. Numerical results are shown in Fig. 9. As expected, the relative error of the Jacobi coefficients decreases as M increases and we can choose a large M such that the relative error of the coefficients remains smaller than a given tolerance.

Example 9.2. We consider the function $f(x) = \frac{x+1}{x^2+a^2}$, which has a pair of complex poles. Relative errors of the first 100 Jacobi coefficients with $\alpha = 1$ and $\beta = 0$ are given for several values of a and M. These Chebyshev coefficients are computed by the trapezoidal rule (3.1) with the optimal radius (3.24) and the number of points in the trapezoidal rule chosen as in (9.1) and $\epsilon = 10^{-13}$. Numerical results are shown in Fig. 10, which confirms the validity of the optimal radius (3.24) for functions with complex poles.

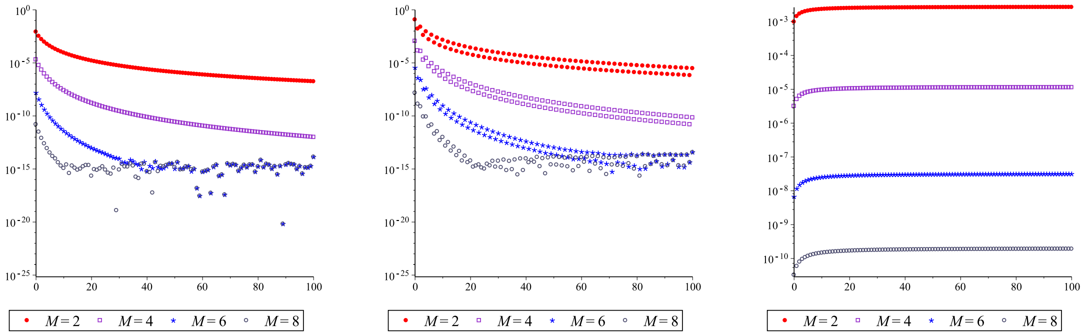

Figure 9: Relative errors of the Jacobi coefficients of $f(x) = e^x$ (left) and $f(x) = \cos(2x+2)$ (middle) and $f(x) = \frac{1}{x-4}$ (right) for several values of M.

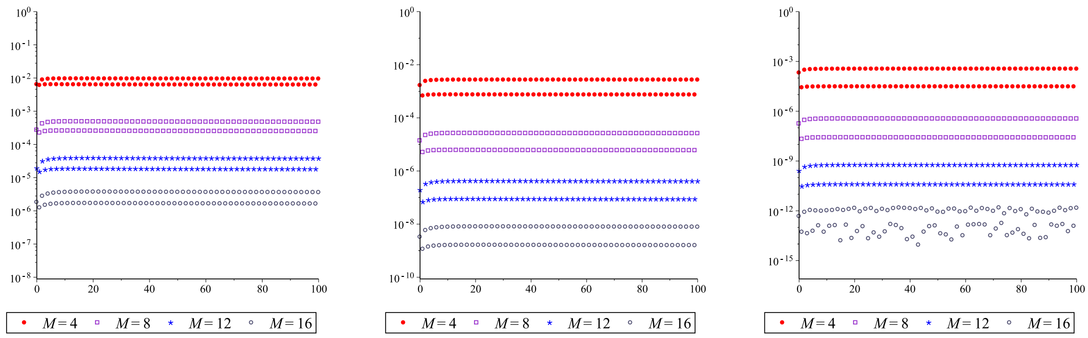

Figure 10: Relative errors of the Jacobi coefficients of $f(x) = \frac{x+1}{x^2+a^2}$ for $a = \frac{1}{2}$ (left) and $a = 1$ (middle) and $a = 2$ (right) for several values of M.

10 Numerical differentiation by spectral expansions

In this section we show some examples to illustrate the accuracy of spectral differentiation based on the spectral expansions.

10.1 Chebyshev spectral differentiation

First, we consider the Chebyshev spectral differentiation. Let

$$f_N^C(x) = \sum_{k=0}^{N}{}' a_k T_k(x)$$

denote the truncated Chebyshev expansion. Then the derivatives of $f(x)$ can be approximated by the corresponding derivatives of $f_N^C(x)$, e.g.

$$f^{(s)}(x) \approx \frac{d^s}{dx^s} f_N^C(x).$$

Let

$$\frac{d^s}{dx^s} f_N^C(x) = \sum_{k=0}^{N} a_k^{(s)} T_k(x).$$

Then the coefficients $a_k^{(s)}$ can be evaluated by using the following recurrence relation [6, p. 498]

$$a_{k-1}^{(s)} = \frac{1}{\delta_{k-1}} \left[a_{k+1}^{(s)} + 2k a_k^{(s-1)} \right], \quad k = N, \ldots, 1,$$

where $a_{N+1}^{(s)} = a_N^{(s)} = 0$ and the coefficients δ_j are defined as

$$\delta_j = \begin{cases} 2, & j = 0, \\ 1, & \text{otherwise.} \end{cases}$$

Moreover, the initial coefficients are given by $a_k^{(0)} = a_k$ for $k \geq 0$.

Example 10.1. We consider the accuracy of the Chebyshev spectral differentiation for the test function $f(x) = e^x$. Each Chebyshev coefficient a_k is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is $m = 100$. In Figure 11 we present the pointwise errors in the evaluation of the s-th order derivative of $f(x)$ by the truncated Chebyshev spectral expansion $f_N^C(x)$. The error is measured at 100 equispaced points in $[-1, 1]$. As can be seen, the error of the Chebyshev spectral differentiation is always very close to machine precision.

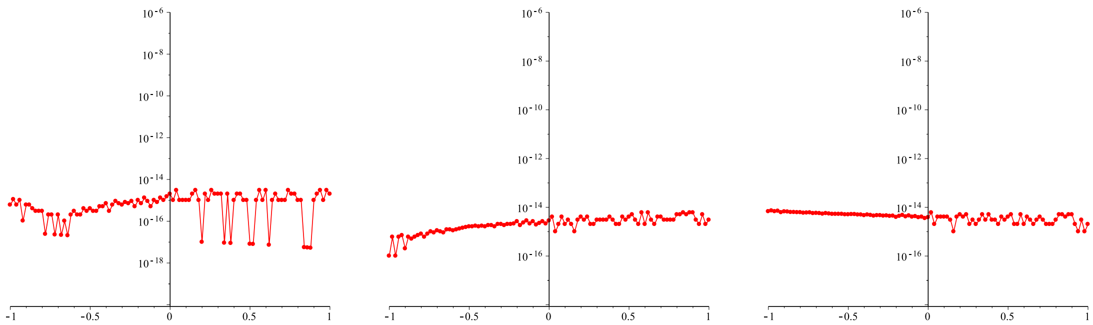

Figure 11: Errors of the s-th order derivative of the truncated Chebyshev expansion $f_N^C(x)$. Here we choose $N = 100$ and $s = 5$ (left), $s = 20$ (middle) and $s = 80$ (right).

Example 10.2. We consider the accuracy of the Chebyshev spectral differentiation for the function $f(x) = \cos(x)$. Each Chebyshev coefficient a_k is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is $m = 100$. In Figure 12 we present the pointwise errors in the evaluation of the s-th order derivative of $f(x)$ by the truncated Chebyshev spectral expansion $f_N^C(x)$.

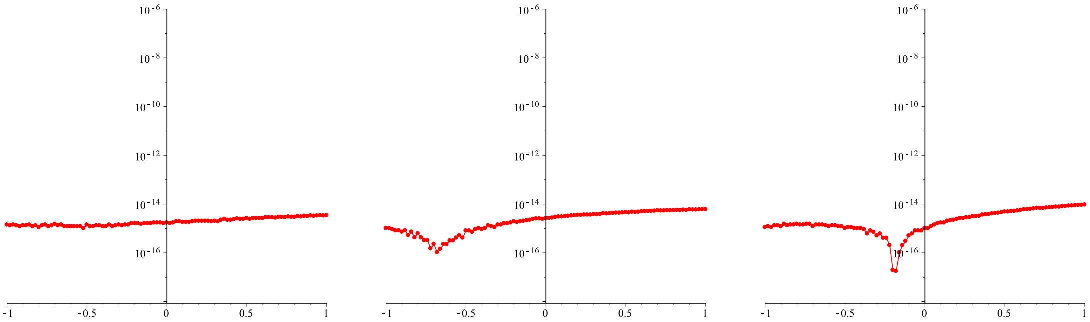

Figure 12: Errors of the s-th order derivative of the truncated Chebyshev expansion $f_N^C(x)$. Here we choose $N = 100$ and $s = 10$ (left), $s = 40$ (middle) and $s = 80$ (right).

Example 10.3. Finally, we consider the accuracy of the Chebyshev spectral differentiation for the test function $f(x) = \frac{x+1}{x^2+4}$. Each Chebyshev coefficient a_k is evaluated by the trapezoidal rule (3.1) with the optimal radius and the number of points in the trapezoidal rule is chosen as in (9.1) and we choose $\epsilon = 10^{-16}$. The pointwise error of the Chebyshev spectral differentiation in the evaluation of the s-th order derivative of $f(x)$ is displayed in Figure 13.

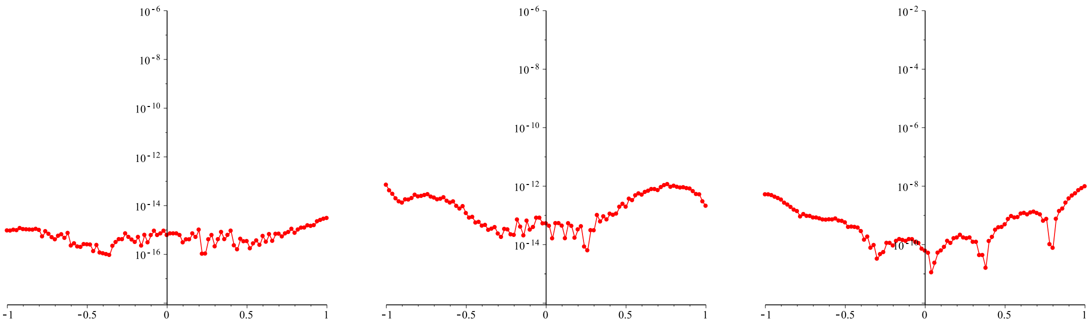

Figure 13: Errors of the s-th order derivative of the truncated Chebyshev expansion $f_N^C(x)$. Here we choose $N = 100$ and $s = 4$ (left), $s = 8$ (middle) and $s = 12$ (right).

10.2 Jacobi spectral differentiation

Finally, we extend the Chebyshev spectral differentiation to the Jacobi case and consider the accuracy of Jacobi spectral differentiation. Let

$$f_N^{(\alpha,\beta)}(x) = \sum_{k=0}^{N} a_k^{(\alpha,\beta)} P_k^{(\alpha,\beta)}(x). \tag{10.1}$$

In analogy to the Chebyshev case, the s-th order derivative of $f(x)$ can be approximated by the s-th order derivative of $f_N^{(\alpha,\beta)}(x)$ and we write it in terms of the Jacobi polynomials

$$f^{(s)}(x) \approx \frac{d^s}{dx^s} f_N^{(\alpha,\beta)}(x) = \sum_{k=0}^{N} a_{k,s}^{(\alpha,\beta)} P_k^{(\alpha,\beta)}(x). \tag{10.2}$$

Then the coefficients $a_{k,s}^{(\alpha,\beta)}$ can be evaluated by using the following recurrence relation [10, Eqn. (8)]

$$\begin{aligned} a_{k-1,s}^{(\alpha,\beta)} = \frac{(2k+\lambda-1)(2k+\lambda-2)}{k+\lambda-1}\Bigg[\frac{1}{2}a_{k,s-1}^{(\alpha,\beta)} + \frac{(k+\alpha+1)(k+\beta+1)}{(2k+\lambda+2)(2k+\lambda+1)(k+\lambda)}a_{k+1,s}^{(\alpha,\beta)} \\ - \frac{\alpha-\beta}{(2k+\lambda+1)(2k+\lambda-1)}a_{k,s}^{(\alpha,\beta)}\Bigg], \quad k = N, \ldots, 1, \end{aligned} \tag{10.3}$$

where $\lambda = \alpha+\beta+1$ and $a_{N+1,s}^{(\alpha,\beta)} = a_{N,s}^{(\alpha,\beta)} = 0$. Moreover, the initial Jacobi coefficients are given by $a_{k,0}^{(\alpha,\beta)} = a_k^{(\alpha,\beta)}$ for $k \geq 0$ and the Jacobi coefficients $a_k^{(\alpha,\beta)}$ are evaluated using the method in §8.

Example 10.4. We consider the accuracy of the Jacobi spectral differentiation for the test function $f(x) = \frac{x+1}{x^2+4}$. The pointwise error of the Jacobi spectral differentiation in the evaluation of the s-th order derivative of $f(x)$ is displayed in Figure 14. We can see that the Jacobi spectral differentiation is accurate for the computation of high-order derivatives. Meanwhile, more accurate approximations are obtained as M increases.

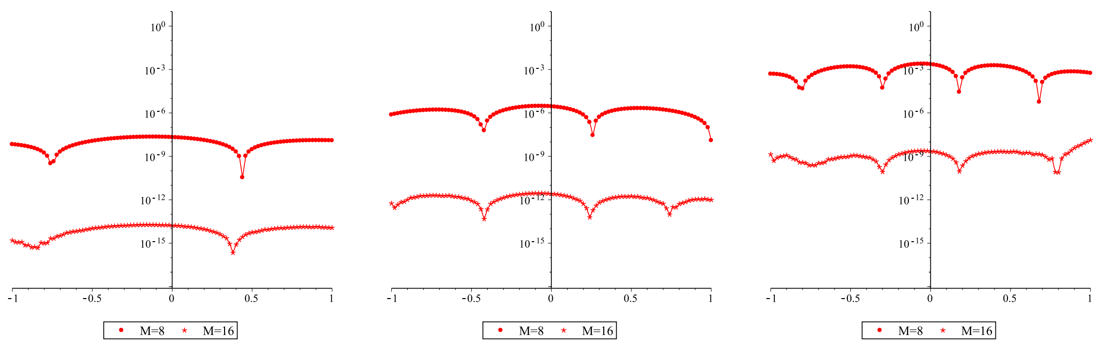

Figure 14: Errors of the s-th order derivative of the truncated Jacobi expansion $f_N^{(1,2)}(x)$. Here we choose $N = 100$ and $s = 4$ (left), $s = 8$ (middle) and $s = 12$ (right).

11 Conclusion

In this paper, we have discussed the computation of spectral expansion coefficients of analytic functions. Two strategies have been proposed based on the computational accuracy and efficiency of spectral coefficients. For the first strategy, we have investigated the computation of Jacobi coefficients by substituting the Chebyshev coefficients into the Jacobi coefficients directly. Truncating the resulting series yields an approximation to the Jacobi coefficients. A three term recurrence relation is established for the computation of the connection coefficients between Jacobi and Chebsyehv polynomials. Finally, we proved that the first N Jacobi expansion coefficients can be computed rapidly with the FFT in $\mathcal{O}(N \log N)$ operations, for a given desired tolerance ϵ.

The second strategy led to an accurate algorithm for computing the spectral coefficients. The starting point of this strategy is the contour integral expression of Chebyshev coefficients. Based on the idea of Bornemann's analysis for the Taylor coefficients, we have shown that an optimal radius exists for each Chebyshev coefficient. Computing each Chebsyehv coefficient with the optimal radius guarantees the relative error to be small. However, this strategy is more expensive, typically $\mathcal{O}(N^2)$ operations for computing the first N Chebyshev coefficients. Similar results were found for the high accuracy computation of Jacobi coefficients.

Finally, we present an accurate numerical differentiation scheme via the Chebyshev spectral expansion. Numerical examples show that the proposed Chebyshev spectral differentiation scheme can provide very accurate approximations to high order derivatives of analytic functions.

A Asymptotic analysis for $\tau_{j,k}^{(\alpha,\beta)}$

Theorem A.1. *Let $\Omega = \{-1, 1, 3, 5, \ldots\}$. For $\alpha, \beta > -1$, if neither 2α nor 2β belongs to Ω, we have*

$$\tau_{j,k}^{(\alpha,\beta)} = \mathcal{O}(j^{-\min\{2\alpha+2,\ 2\beta+2\}}), \quad j \to \infty. \tag{A.1}$$

If one of 2α and 2β belongs to Ω, then

$$\tau_{j,k}^{(\alpha,\beta)} = \begin{cases} \mathcal{O}(j^{-2\beta-2}), & \text{if } 2\alpha \in \Omega, \\ \mathcal{O}(j^{-2\alpha-2}), & \text{if } 2\beta \in \Omega. \end{cases} \tag{A.2}$$

If both 2α and 2β belong to Ω and $2\alpha = 2k_1 - 1$, $2\beta = 2k_2 - 1$, for $k_1, k_2 \geq 0$, then

$$\tau_{j,k}^{(\alpha,\beta)} = 0, \quad j \geq k + k_1 + k_2 + 1. \tag{A.3}$$

Proof. First, make a change of variable $x = \cos\theta$ yields

$$\begin{aligned} h_k^{(\alpha,\beta)} \tau_{j,k}^{(\alpha,\beta)} &= \int_{-1}^{1} \omega^{(\alpha,\beta)}(x) P_k^{(\alpha,\beta)}(x) T_j(x) dx \\ &= \int_0^{\pi} \theta^{2\alpha+1} (\pi - \theta)^{2\beta+1} g(\theta) \cos(j\theta) d\theta \end{aligned}$$

where

$$g(\theta) = 2^{\alpha+\beta+1} (\theta^{-1} \sin \tfrac{\theta}{2})^{2\alpha+1} ((\pi - \theta)^{-1} \cos \tfrac{\theta}{2})^{2\beta+1} P_k^{(\alpha,\beta)}(\theta).$$

It is clear that $\min\{2\alpha+1, 2\beta+1\} > -1$. Let

$$\psi(\theta) = (\pi-\theta)^{2\beta+1} g(\theta), \quad \phi(\theta) = \theta^{2\alpha+1} g(\theta). \tag{A.4}$$

We observe that $\psi(\theta)$ and $\phi(\theta)$ are regular at $\theta = 0$ and $\theta = \pi$, respectively. Furthermore, straightforward calculation confirms that

$$\psi^{(2s+1)}(0) = 0, \quad \phi^{(2s+1)}(\pi) = 0, \quad s \geq 0. \tag{A.5}$$

Combining these with lemma 5.8, we have that for large j,

$$\begin{aligned} h_k^{(\alpha,\beta)} \tau_{j,k}^{(\alpha,\beta)} &= \int_0^\pi \theta^{2\alpha+1}(\pi-\theta)^{2\beta+1} g(\theta)\cos(j\theta)d\theta \\ &\sim \cos(\alpha\pi)\sum_{s=0}^{\infty}(-1)^{s+1}\frac{\psi^{(2s)}(0)\Gamma(2s+2\alpha+2)}{j^{2s+2\alpha+2}(2s)!} \\ &\quad - (-1)^j\cos(\beta\pi)\sum_{s=0}^{\infty}(-1)^{s}\frac{\phi^{(2s)}(\pi)\Gamma(2s+2\beta+2)}{j^{2s+2\beta+2}(2s)!}. \end{aligned} \tag{A.6}$$

To derive the asymptotic of $\tau_{j,k}^{(\alpha,\beta)}$, we will distinguish three cases. First, if neither 2α nor 2β belongs to Ω, then (A.1) follows immediately from the above expansion. Second, if either 2α or 2β belongs to Ω, then by noting that $\cos(\frac{k}{2}\pi) = 0$ for $k \in \Omega$, the result (A.2) follows. Finally, if both 2α and 2β belong to Ω. For simplicity, we suppose $2\alpha = 2k_1 - 1$ and $2\beta = 2k_2 - 1$ with $k_1, k_2 \geq 0$. Thus we can write $\tau_{j,k}^{(\alpha,\beta)}$ as

$$h_k^{(\alpha,\beta)} \tau_{j,k}^{(\alpha,\beta)} = \int_{-1}^{1} \frac{T_j(x)(1-x)^{k_1}(1+x)^{k_2}}{\sqrt{1-x^2}} P_k^{(\alpha,\beta)}(x)dx.$$

It is well known that $T_j(x)(1-x)^{k_1}(1+x)^{k_2}$ can be written as a linear combination of $\{T_s\}$ for $j - k_1 - k_2 \leq s \leq j + k_1 + k_2$. Therefore, if $j \geq k + k_1 + k_2 + 1$, the last assertion follows by using the orthogonality of the Chebyshev polynomials of the first kind. This completes the proof. □

B Computational complexity of Algorithm 2

In analogy to the case of Algorithm 1, we can choose a constant M independent of N so that Algorithm 2 is also an $\mathcal{O}(N \log N)$ algorithm.

Theorem B.1. *Given a tolerance ϵ, there exist a constant M independent of N such that*

$$|a_k^{(\alpha,\beta)} - \tilde{a}_k^{(\alpha,\beta)}| < \epsilon, \quad k \geq 0.$$

Proof. We first consider the case $k = 0$. Using (4.10) and (5.31), it holds that

$$\begin{aligned}
|a_0^{(\alpha,\beta)} - \tilde{a}_0^{(\alpha,\beta)}| &\leq \sum_{m=M+1}^{\infty} |b_m \sigma_{m,0}^{(\alpha,\beta)}| \\
&\leq \zeta \sum_{m=M+1}^{\infty} \frac{m+1}{\rho^m} \\
&= \frac{\zeta((M+1)(1-\rho^{-1})+1)}{\rho^{M+1}(1-\rho^{-1})^2} \\
&< \frac{\zeta(M+2)}{(1-\rho^{-1})^2 \rho^{M+1}}. \qquad \text{(B.1)}
\end{aligned}$$

where $\zeta = \frac{\mathcal{M}L(\mathcal{E}_\rho)}{\pi\rho}$. For $k \geq 1$, using Lemma 6.1 and (5.31), we have

$$\begin{aligned}
|a_k^{(\alpha,\beta)} - \tilde{a}_k^{(\alpha,\beta)}| &\leq \sum_{m=M+1}^{\infty} |b_{k+m} \sigma_{k+m,k}^{(\alpha,\beta)}| \\
&\leq \zeta \sum_{m=M+1}^{\infty} \frac{k+m+1}{\rho^{k+m}} \sqrt{\frac{h_0^{(\alpha,\beta)}}{h_k^{(\alpha,\beta)}}} \\
&\leq \sqrt{Ck}\zeta \sum_{m=M+1}^{\infty} \frac{k+m+1}{\rho^{k+m}} \\
&= \sqrt{Ck}\zeta \frac{(k+M+1)(1-\rho^{-1})+1}{\rho^{k+M+1}(1-\rho^{-1})^2} \\
&\leq \sqrt{Ck}\zeta \frac{k+M+2}{\rho^{k+M+1}(1-\rho^{-1})^2}. \qquad \text{(B.2)}
\end{aligned}$$

For $k \geq 1$, we easily obtain

$$\begin{aligned}
\frac{\sqrt{k}(k+M+2)}{\rho^k} &= (M+2)\frac{\sqrt{k}}{\rho^k} + \frac{k^{\frac{3}{2}}}{\rho^k} \\
&\leq (M+2)\frac{d_1^{\frac{1}{2}}}{\rho^{d_1}} + \frac{d_2^{\frac{3}{2}}}{\rho^{d_2}} \\
&\leq \hat{C}(M+3), \qquad \text{(B.3)}
\end{aligned}$$

where $d_1 = \max\left\{1, \frac{1}{2\log\rho}\right\}$, $d_2 = \max\left\{1, \frac{3}{2\log\rho}\right\}$ and $\hat{C} = \max\left\{\frac{d_1^{\frac{1}{2}}}{\rho^{d_1}}, \frac{d_2^{\frac{3}{2}}}{\rho^{d_2}}\right\}$. Thus, for $k \geq 0$, we obtain the following uniform upper bound

$$|a_k^{(\alpha,\beta)} - \tilde{a}_k^{(\alpha,\beta)}| \leq \frac{\tilde{C}(M+3)}{\rho^{M+1}(1-\rho^{-1})^2}, \qquad \text{(B.4)}$$

where $\tilde{C} = \max\{1, \sqrt{C}\hat{C}\}$. Then it is enough to choose

$$M > -3 - \frac{W(-\frac{(1-\rho^{-1})^2 \log \rho}{\rho^2 \tilde{C}} \epsilon)}{\log \rho}, \tag{B.5}$$

where $W(z)$ is the Lambert function which is defined by $W(z)e^{W(z)} = z$ and we choose the branch $W(x) \leq W(-\frac{1}{e})$ on $(-\frac{1}{e}, 0)$. Under this condition we obtain

$$|a_k^{(\alpha,\beta)} - \tilde{a}_k^{(\alpha,\beta)}| \leq \epsilon, \quad k \geq 0.$$

This completes the proof. □

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